International Centre for Diffraction Data
TECHNICAL COMMITTEE MEETING MINUTES
Thursday, 26 March 2015
9:00 a.m.-12:30 noon
Conference Room A
Matteo Leoni, Chairman

1. Call to Order and Opening Remarks - Matteo Leoni

2. Roll Call and Attendance (on record at ICDD)

3. Additions and/or Deletions to the Agenda - Matteo Leoni

4. Approval of the 2014 Minutes - Matteo Leoni

   Motion 1: Wallace moved to approve the 2014 Technical Committee minutes. Seconded by Fawcett.

   Motion passed. 28 Yes, 0 No, 0 Abstain

5. Scholarship Recipient Presentation - Benjamin Trump

6. Reports/Presentations of Technical Regional Co-Chairs and International Guests

   A. China - Xiaolong Chen (not present) Fawcett's presentation
   B. Eastern Pacific Rim - Takashi Ida
   C. European Community - Matteo Leoni
   D. Indian Ocean Rim - Vanessa Peterson (not present and no report)
   E. Newly Independent States - Evgeny Antipov
   F. North America - John Anzelmo (not present) Maguire's presentation
   G. South America - Miguel Delgado
   H. United Kingdom - David Rendle

Break at 10:55-11:10 a.m.

7. Subcommittee Reports and Motions (my recorded motions with votes:

   A. Materials
      1) Ceramics - Peter Zavalij
      2) Metals and Alloys - Pete Wallace

   Motion 2: The Metals &Alloys Subcommittee recommends to the Technical Committee that the ***M&A Standard*** *empirical formula, space group, Z, Wyckoff sequence* be made available to PDF4+ users.

   Note: *M&A Standards* are based upon the accepted Linus Pauling File (LPF) prototype structure for each material.

   Wallace moved. Dann seconded.
   Motion passed. 28 Yes, 0 No, 0 Abstain

   Motion 3: The Metals & Alloys Subcommittee recommends to the Technical Committee that structural information (e.g., prototype structure and Pearson Symbols) located under the *Miscellaneous* tab of PDF4+ be relocated to the *Structure or a new Structure-II* tab when possible.

   Wallace moved. Dann seconded.
   Motion passed. 29 Yes, 0 No, 0 Abstain

3) Micro and Meso - Sue Quick

Motion 4: The Micro and Meso Subcommittee recommends to the Technical Committee that ICDD headquarters explore programs to characterize pore size for micro/mesoporous materials. An example program is TOPOS.

Discussion: T. Blanton requests that a task group decide if this is useful and determine what needs to be done. Blatov program mentioned, free for personal use, not commercial.

Quick moved. Seconded: Dann seconded.
Motion passed. 24 Yes, 0 No, 3 Abstain

4) Minerals - Jim Kaduk
5) Organic and Pharmaceutical - Fred Wireko

Motion 5: The Organic and Pharmaceutical Subcommittee recommends to the Technical Committee that ICDD evaluate the ability of 2D chemical structure and fragment search capability.

Wireko moved. Wallace seconded.
Motion passed. 28 Yes, 0 No, 0 Abstain

6) Polymers - Lizhi Liu

B. Characterization Methods and Tools

1) Electron Diffraction - Bryan Wheaton
Tutorial electron diffraction frequently viewed on website. Bulletin received over 200 views.

2) Non-Ambient Diffraction - Andrew Payzant

Motion 6: The Non-Ambient Subcommittee recommends to the Technical Committee that the ICDD provide logistical support for quarterly teleconference meetings of the Non-Ambient Subcommittee members.

Payzant moved. Hubbard seconded.
Motion passed. 28 Yes, 0 No, 0 Abstain

Motion 7: The Non-Ambient Subcommittee recommends to the Technical Committee that the non-ambient parameter have not only a constant field but a parametric equation and range of application to enable future functionality of the database.

Payzant moved. Wallace seconded.
Motion passed. 30 Yes, 0 No, 0 Abstain

Payzant commented that some of the videos no longer work, and often they are truncated. ICDD needs to work on it.

3) Synchrotron & Neutron Scattering Methods - Pamela Whitfield

Motion 8: The Synchrotron & Neutron Scattering Subcommittee recommends to the Technical Committee that funding be provided for John Faber to continue his efforts in implementing search-match for neutron time-of-flight (TOF) data.

Whitfield moved. Blanton seconded.
Motion passed. 36 Yes, 0 No, 2 Abstain (Faber by name)

Motion 9: The Synchrotron & Neutron Scattering Subcommittee recommends to the Technical Committee that the ICDD support efforts to capture additional information such as magnetic structures (including transition temperatures) from neutron-derived structures and experimental data.

Whitfield moved. Hubbard seconded.
Motion passed. 35 Yes, 0 No, 0 Abstain

4) X-ray Diffraction Methods - Robert Papoular/Chris Gilmore
5) X-ray Fluorescence - Mark Rodriguez

Motion 10: The XRF Subcommittee recommends to the Technical Committee that a test of the databased be performed wherein X-ray Fluorescence composition results from a series of common compounds and/or minerals be processed through the *Composition field* of the *Elements* tab. The test of these known single phase materials (perhaps 50-100 "common phases" in the PDF database) would assess the effectiveness of the database to perform phase identification from XRF results alone. A report would be generated by ICDD to document how well the identification process worked, as well as possible recommendations for improved means of identification. With a request that a report would be completed by the Fall Board 2015 meeting.

Rodriguez moved. Hubbard seconded.
Motion passed. 32 Yes, 0 No, 0 Abstain

Fawcett: Analysis certified materials would help. Get the data on the web, per Taylor. Gilmore commented that XRD and XRF together in soil analysis is highly useful and encouraged this motion tremendously.

Motion 11: The XRF Subcommittee recommends to the Technical Committee that newly determined (updated) Fundamental Parameters (FP) values be obtained and archived by ICDD for the benefit of XRF experimentalists, equipment manufacturers, and future ICDD projects requiring accurate FP tabulations.

Initial collaborative discussions have been established with Michael Mantler (U. Vienna).

Rodriguez moved. Wallace seconded.
Motion passed. 33 Yes, 0 No, 0 Abstain

Perhaps compiling could be outsourced. Archiving is the critical issue.

Motion 12: New X-ray Fluorescence Subcommittee Mission Statement

The X-ray Fluorescence Subcommittee will provide recommendations for X-ray Fluorescence to be a complement to both the PDF and ICDD. This entails synergistic interchange between data collected from XRD and XRF:

- Use of chemical composition to support powder diffraction analysis.
- Ability to improve chemical composition by use of the powder diffraction
- To ultimately obtain simulated XRF data as a means of material analysis validation such as refinement of data from multiple analytical methods.

In addition, the subcommittee shall develop new educational opportunities for ICDD and offer guidance on addressing elemental composition issues which are of strategic interest to ICDD.

Taylor moved. Hubbard seconded.
Motion passed. 35 Yes, 0 No, 0 Abstain

C. ICDD Activities
   1) Education - Carlo Segre
   2) PDF Editorial Staff - Soorya Kabekkodu
      Quality marks of the future were mentioned as a future discussion topic.

8. New Business - Matteo Leoni

9. Adjournment

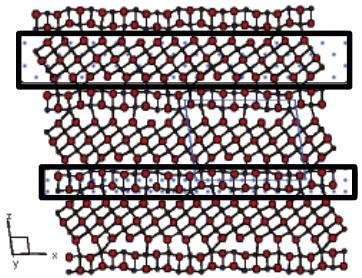
Structural Determination of New Iridate Compounds

Benjamin A. Trump
McQueen Lab
Institute for Quantum Matter
Department of Chemistry
Johns Hopkins University

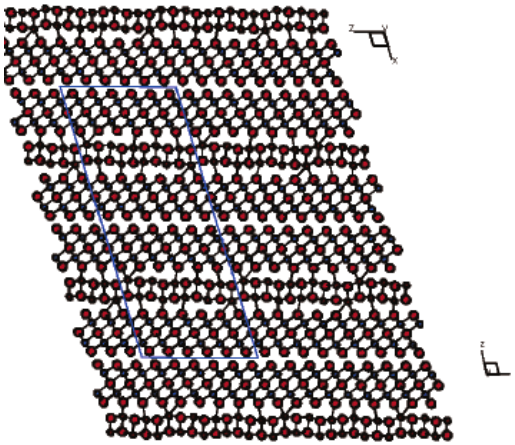
Background – Homologous Series

$(PbSe)_{3m}(Bi_2Se_3)_{5n}$

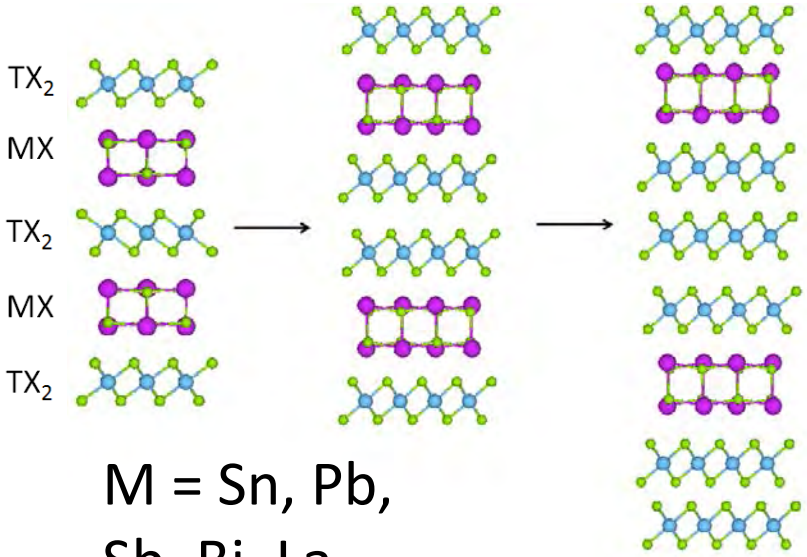
1:1



1:2



$(MX)_{1+\delta}(TX_2)_n$



M = Sn, Pb, Sb, Bi, La

T = Ti, V, Cr, Nb, Ta

X = S, Se, Te

Previously:

M = Bi

T = Ti

X = Se

n = 1, 2

Trump, B.A. et al. *J. Sol. St. Chem.* **209**, 6-12 (2014).

Current:

M = Sn

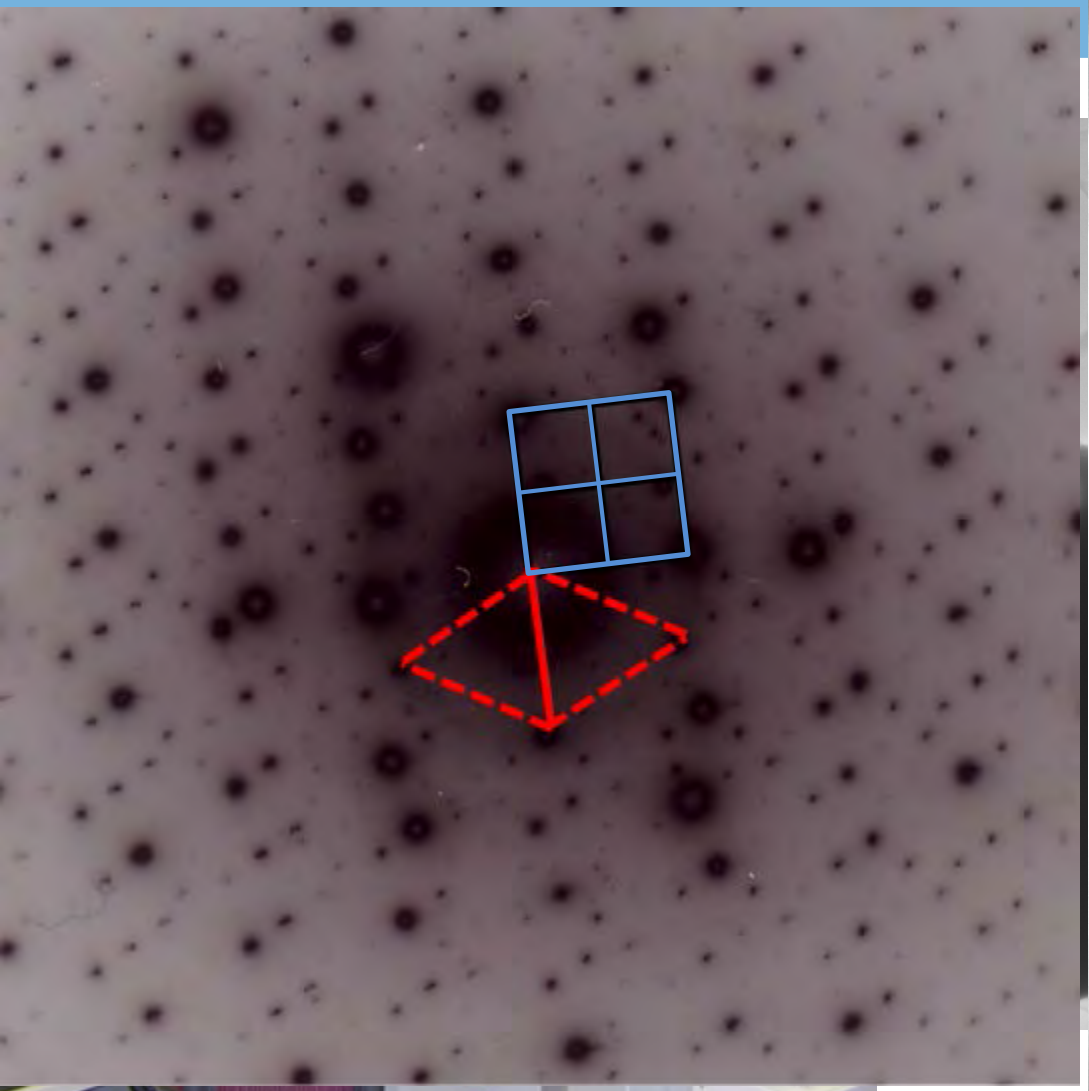
T = Ir?

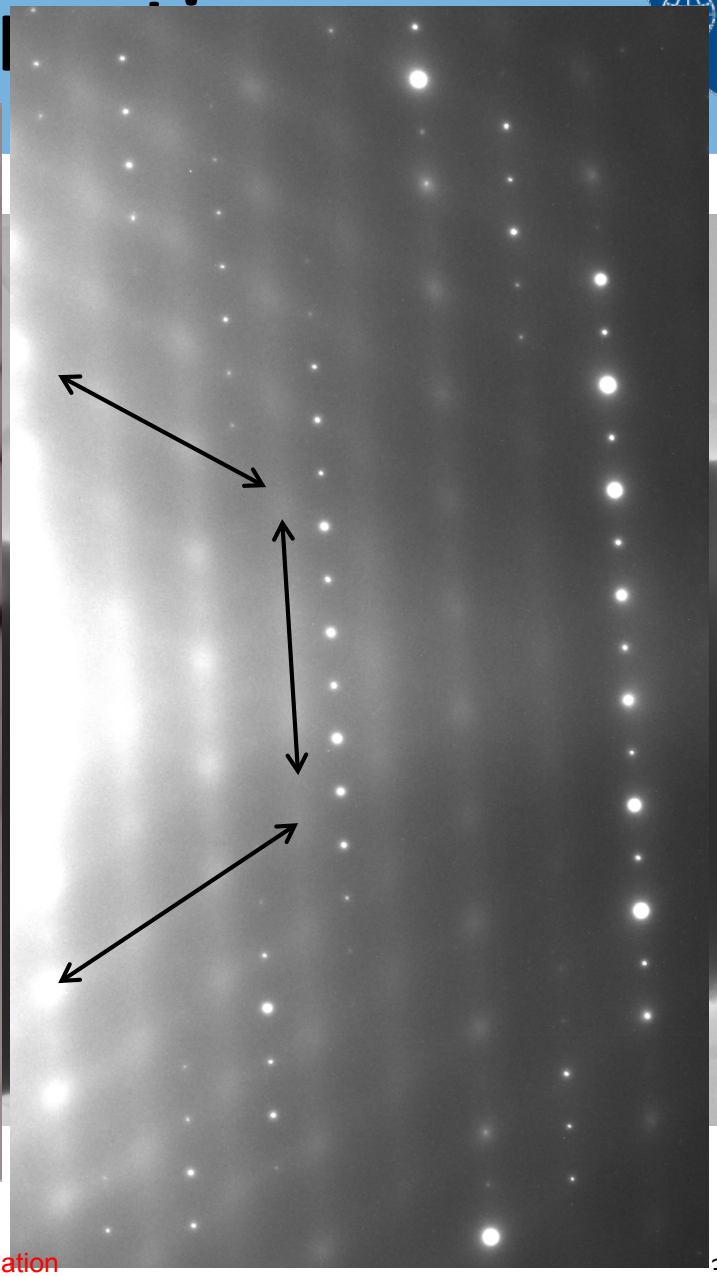
X = Se

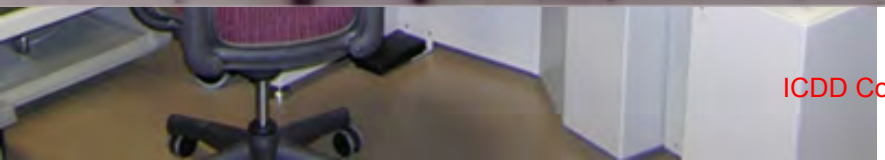
Wiegers, G.A., *Prog. Solid St. Chem.* **24**, 1-139 (1996).

Kanatzidis, M., *Acc. Chem. Res.* **38**, 361-370 (2005).

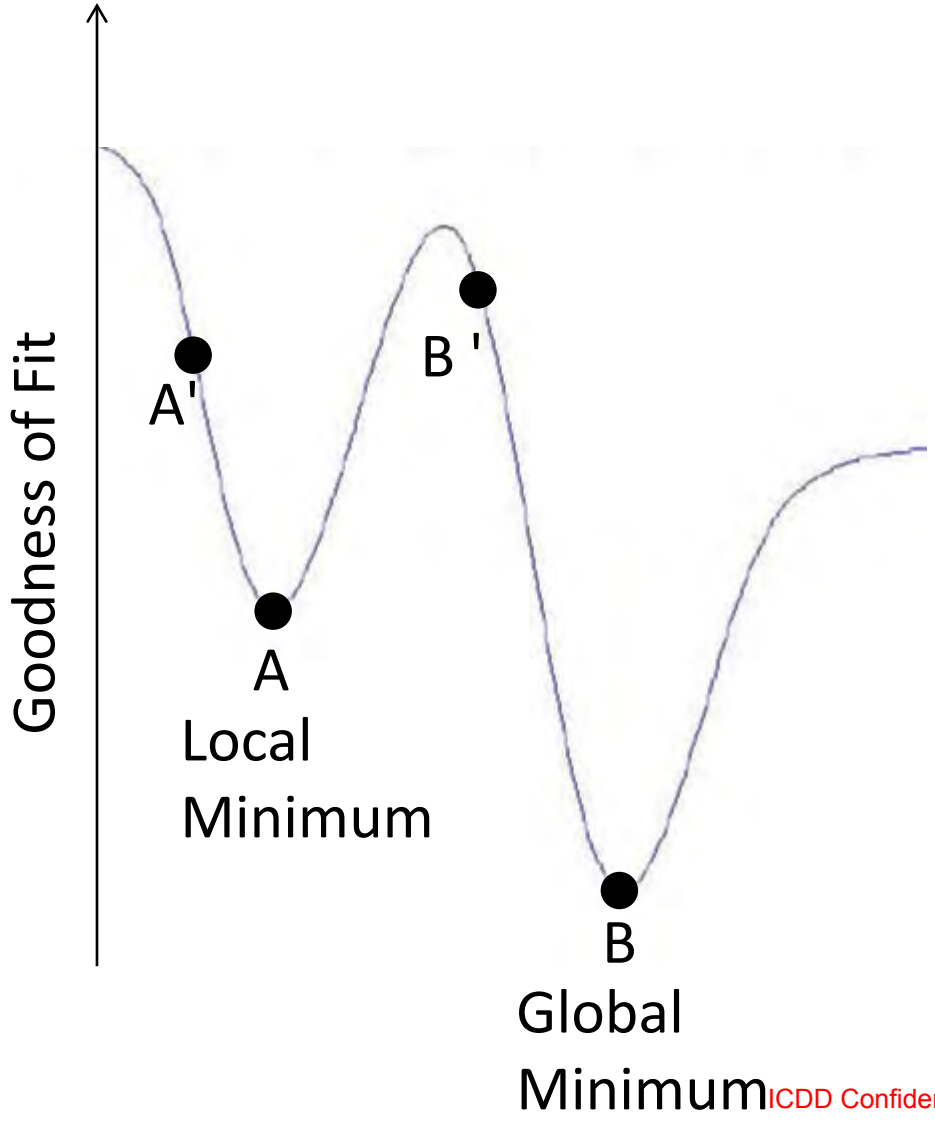
Electron Diffr





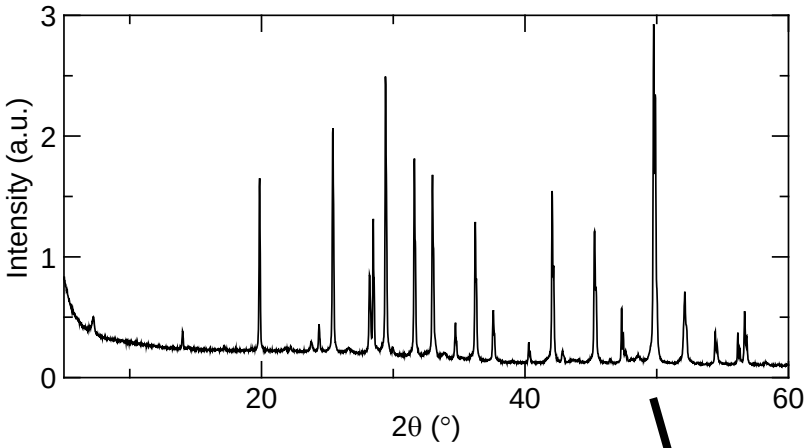


Simulated Annealing (SA)

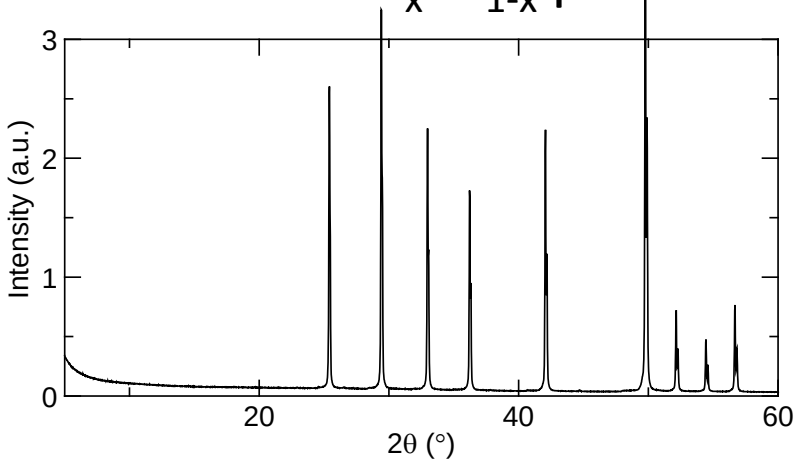


- Uses a temperature (*T)* as a variable
- Starts by randomly changing a variable
- Then refines and chooses if fit is better or worse – or similar based on probability – larger *T*, larger probability
- Allows for finding Global Minimum

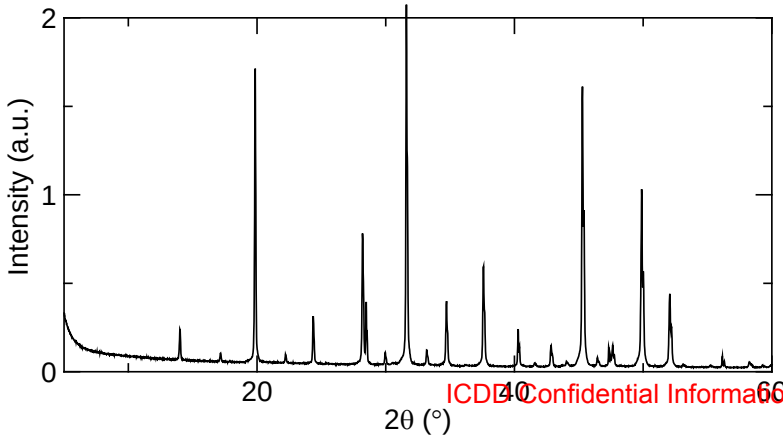
Case Study: Initial Work



$Pa\bar{3}$ – $IrSn_xSe_{1-x}$ phase



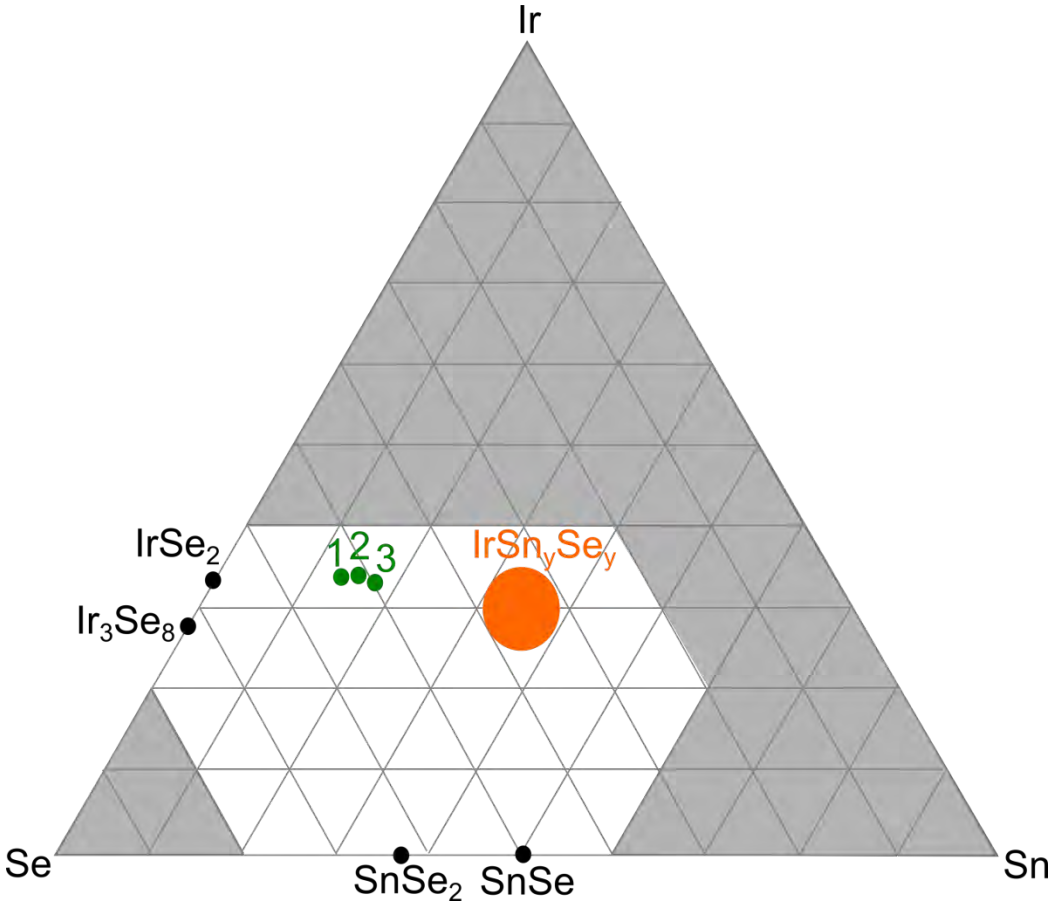
$Im\bar{3}$ – $IrSn_ySe_y$ phase



Problems:

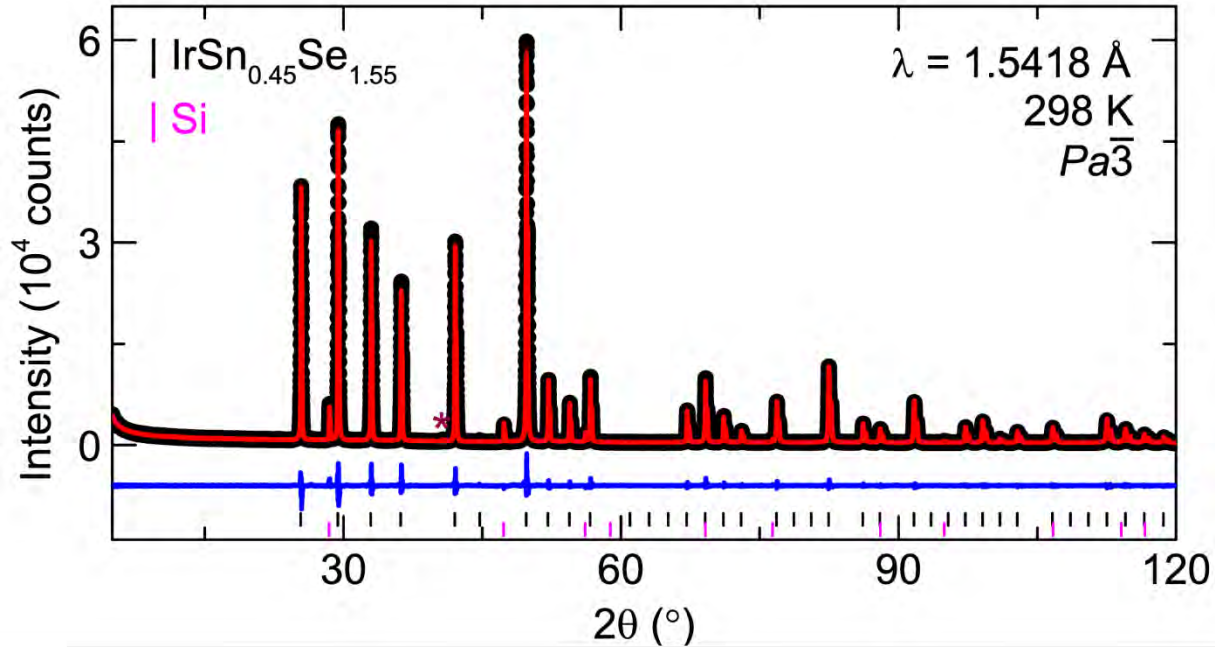
- Formula?
- Unit Cells?
- Spacegroups?
- Atomic Positions?

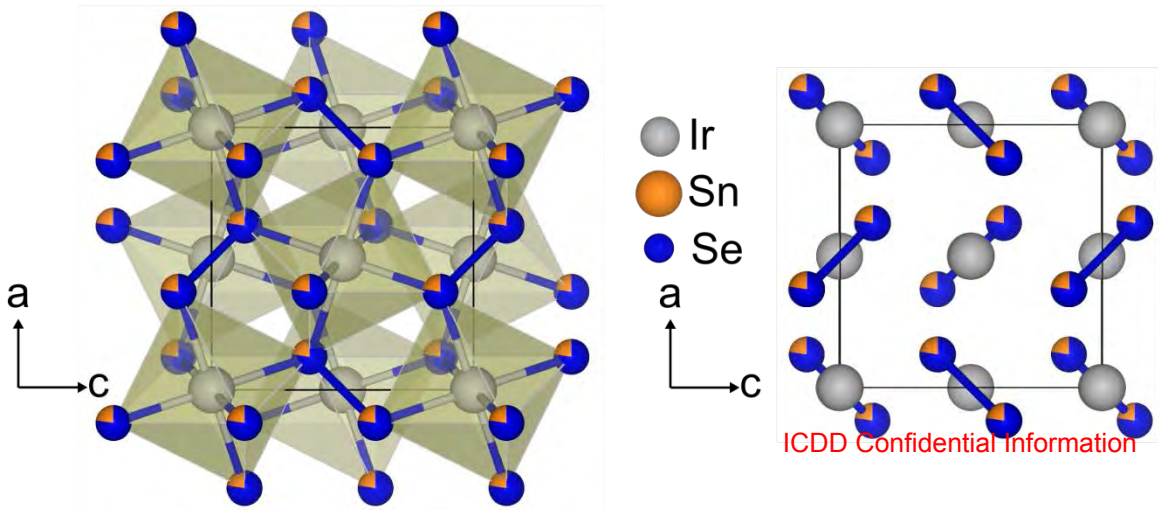
Formula for $IrSn_xSe_{2-x}$



- 1 – $IrSn_{0.4}Se_{1.6}$ leads to 12 wt% IrSe2 impurity
- 2 – $IrSn_{0.45}Se_{1.55}$ has no impurities
- 3 – $IrSn_{0.5}Se_{1.5}$ leads to 21 wt% $IrSn_ySe_y$ impurity

Refinement of $IrSn_{0.45}Se_{1.55}$



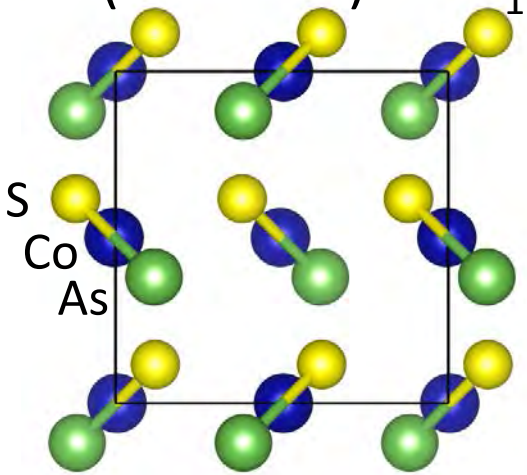


Formally written as:

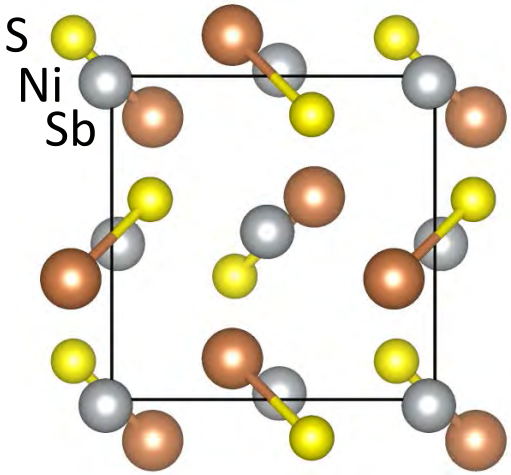
$Ir^{3+}_2(SnSe)^{4-}(Se_2)^{2-}$

Double Checking $IrSn_{0.45}Se_{1.55}$

CoAsS (cobaltite) $Pca2_1$ (29)



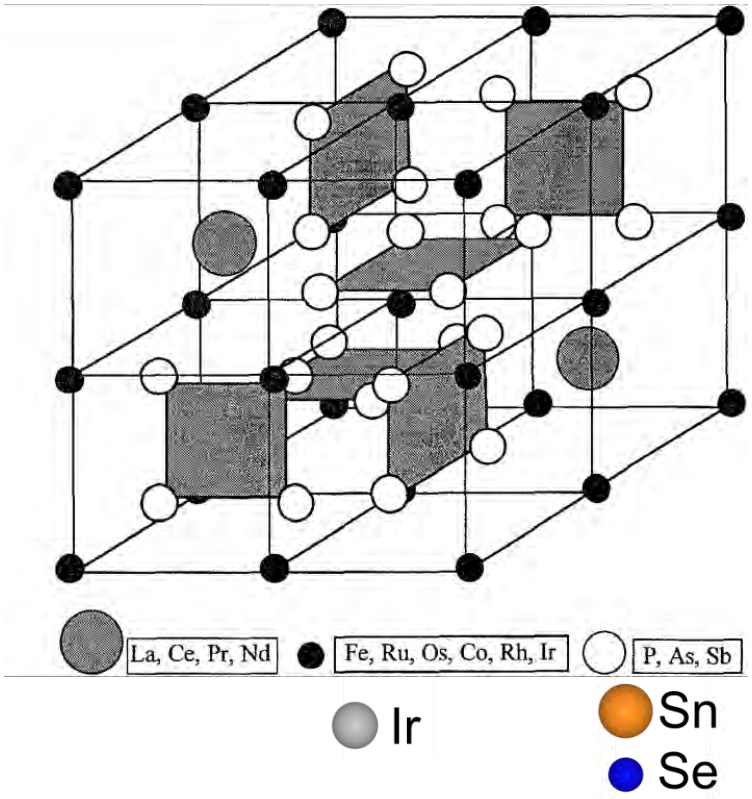
NiSSb (ullmannite) $P2_13$ (198)

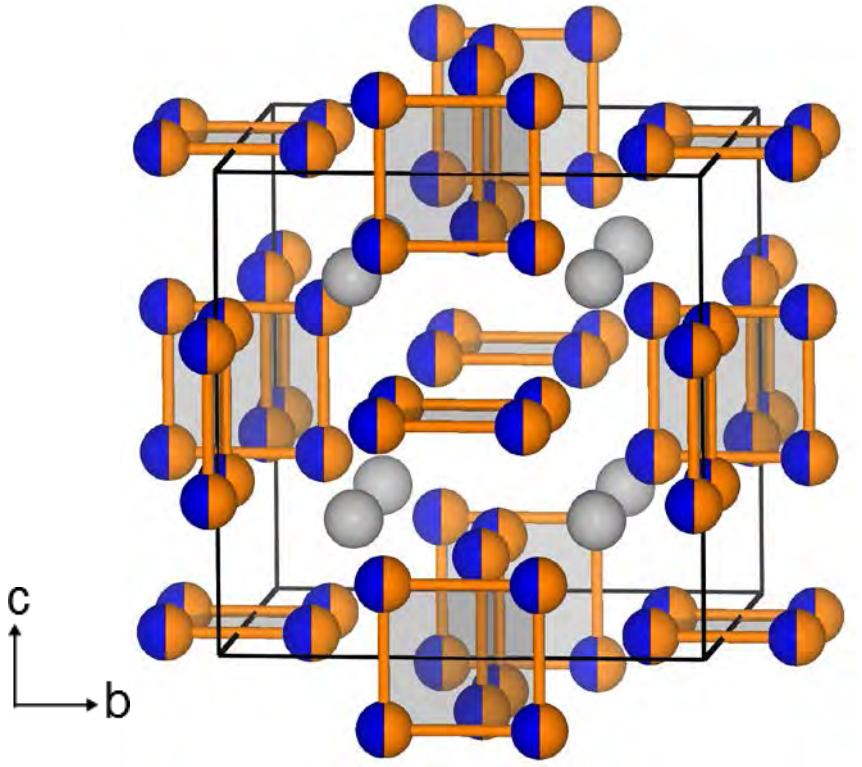


- Pyrite structure with multiple anions often orders to lower symmetry
- Can distinguish by allowed reflections
- $P2_13$ allows *h* odd for (*h*00)
- $Pca2_1$ allows *h or k* odd for (*hk*0)
- We do not observe (100) or (110) reflections hence Sn is not ordered!

Baylis, P. *American Mineralogist* **67** 1048-57 (1982).
Ramsdell, L.S. *American Mineralogist* **10** 281-301 (1925).

$Ir_2Sn_3Se_3$ – Simulated Annealing

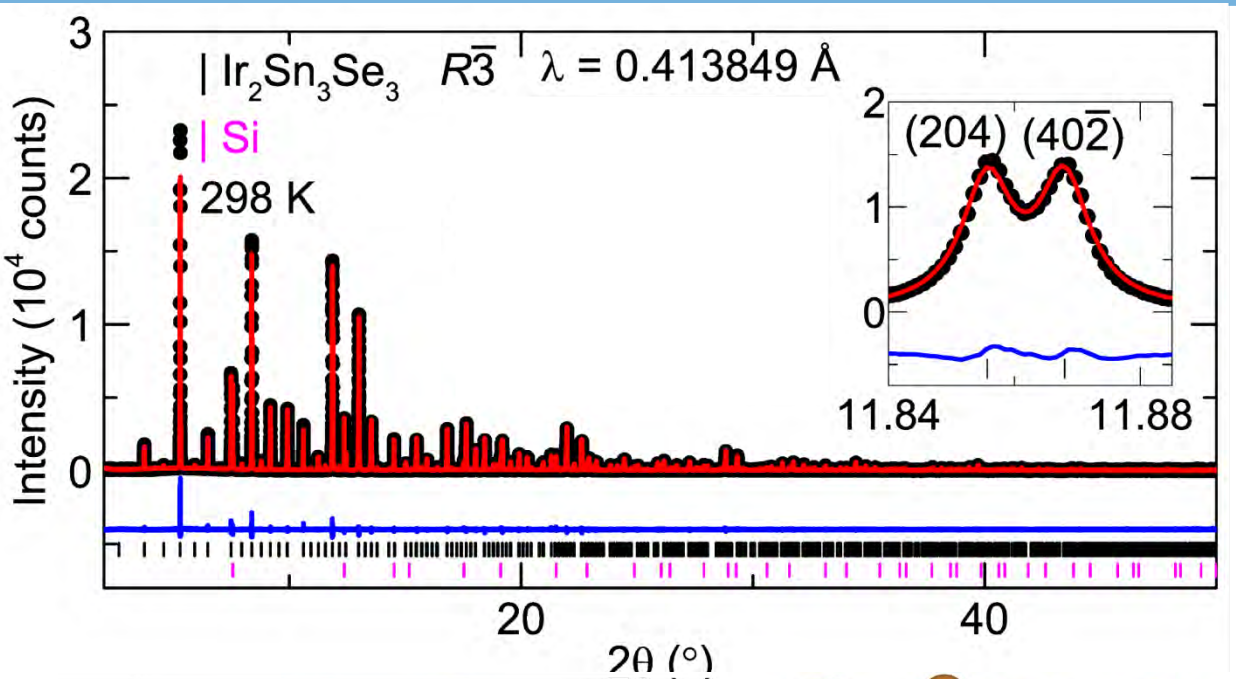


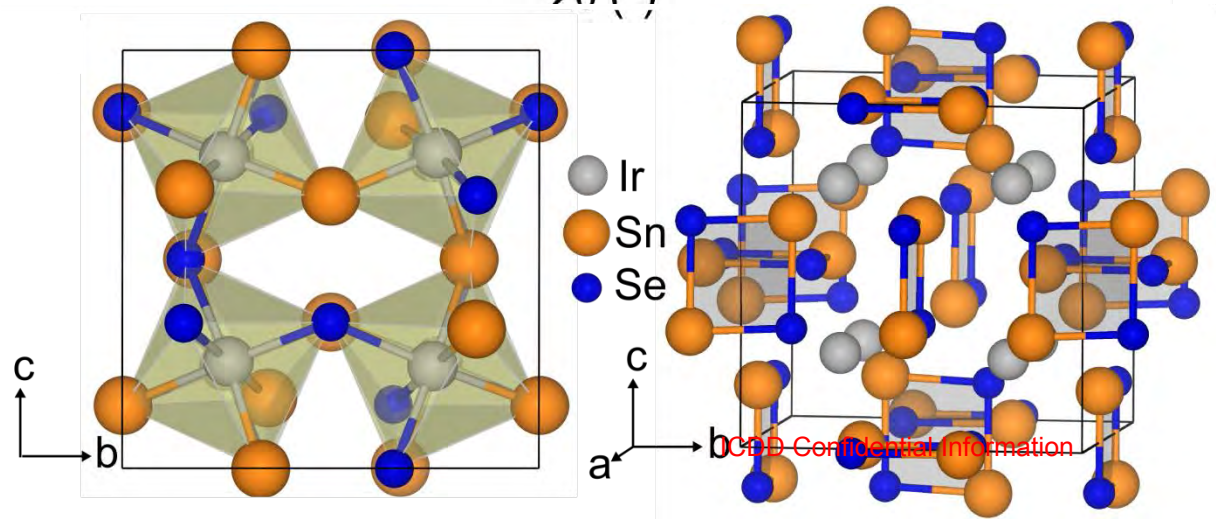


- Initial Simulated Annealing was using *Im*$\bar{3}$ model (204) by letting Sn and Se occupancies refine – led to mixing of sites

Fleurial J.-P. et al. *16th Intern. Conf. on Thermoelectrics* 1-11 (1997).

Refinement of $Ir_2Sn_3Se_3$



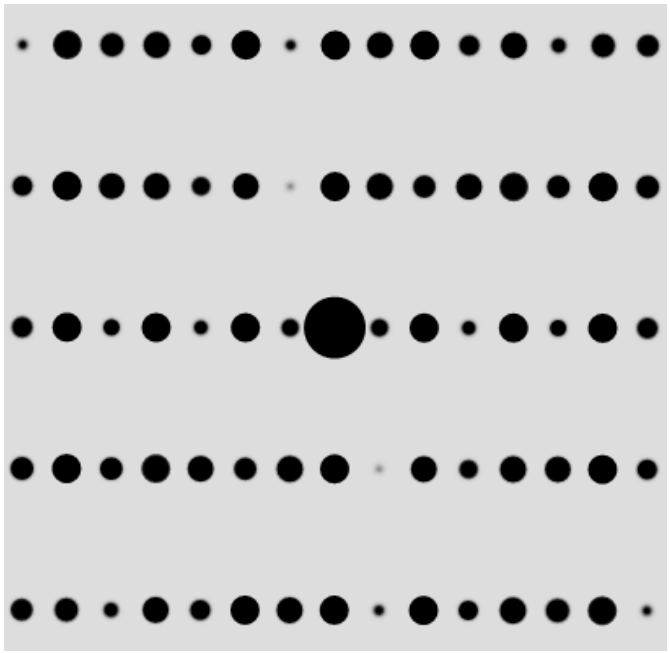


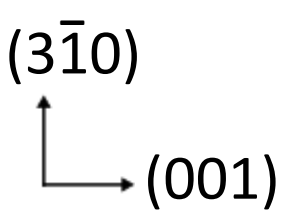
Formally written as:

$Ir^{3+}_4(Sn_2Se_2)^{4-}_3$

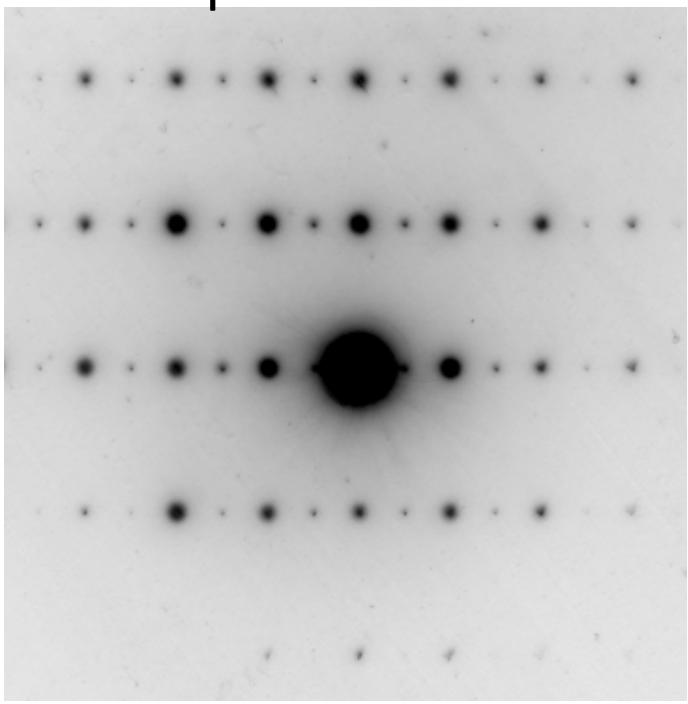
Double checking $Ir_2Sn_3Se_3$

Simulated with SingleCrystal



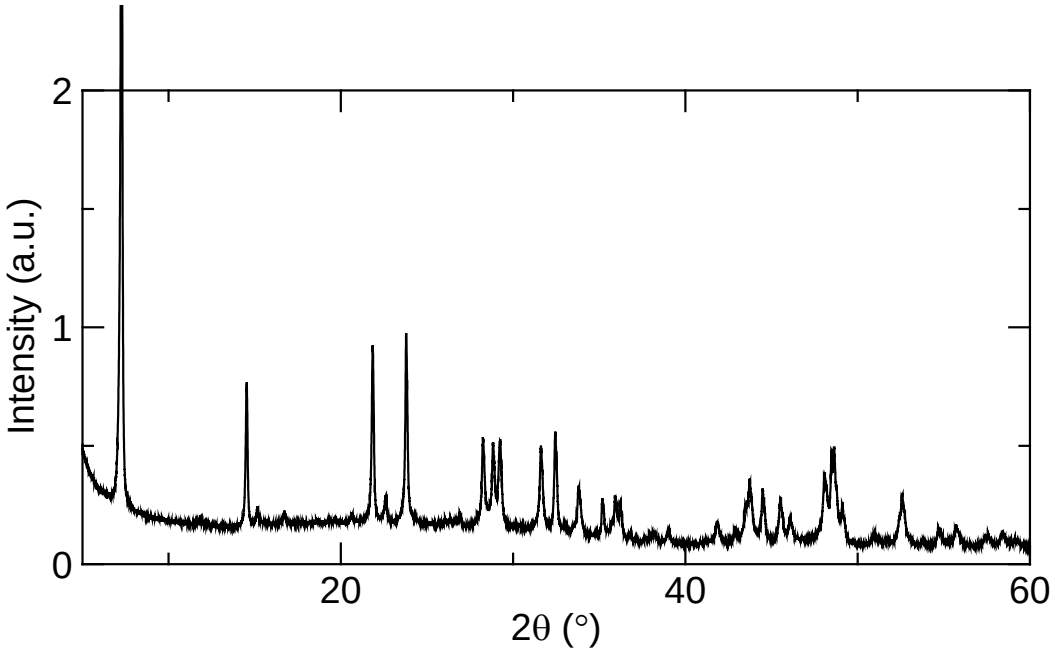


Experimental

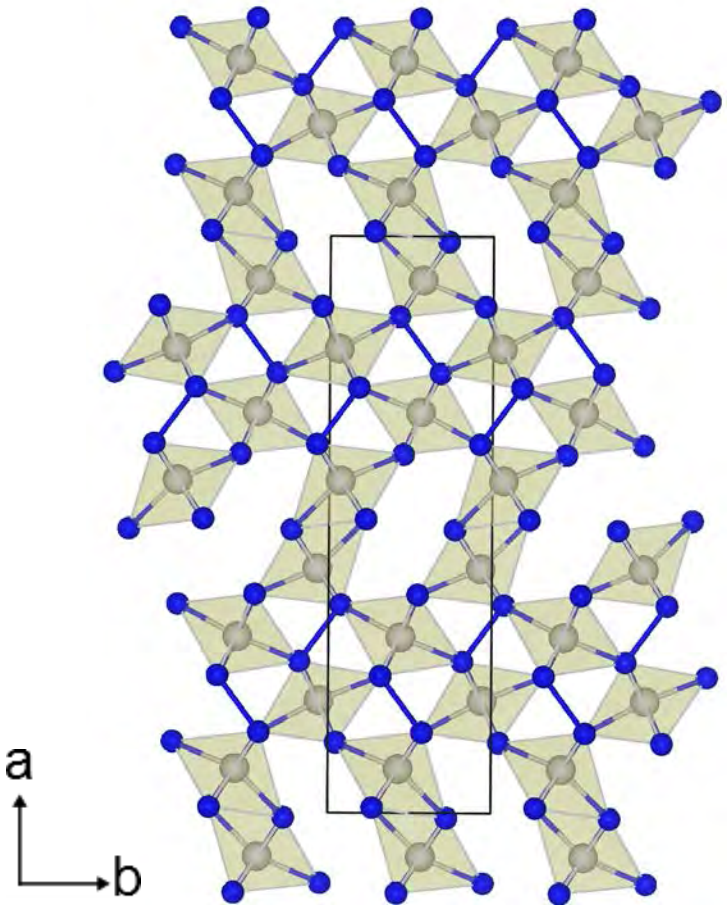


- No evidence for doubling of unit cell in any direction
- Pattern matches well for <3$\bar{1}$0> zone axis of $R\bar{3}$ $Ir_2Sn_3Se_3$

Ir-Sn-Se Mystery Phase



$IrSe_2$



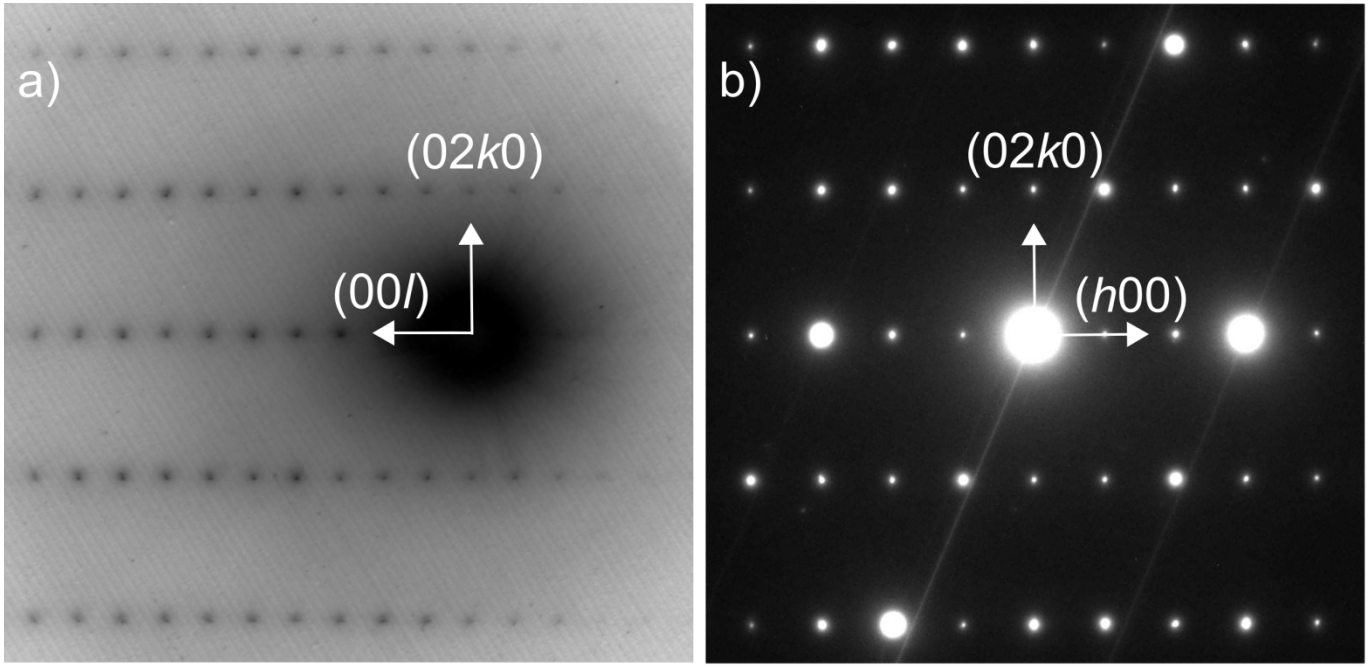
- Unknown formula
- Best guess: $(IrSe_2)_xSn_ySe_z$

x = 1-2 y = 1-2 z = 1-2

- Layered compound
- Similar to $IrSe_2$?

Jobic, S. et al. *Inorg. Chem.* **39** 4370-4373 (2000).

Ir-Sn-Se SAED



- Experimentally observed lattice of:

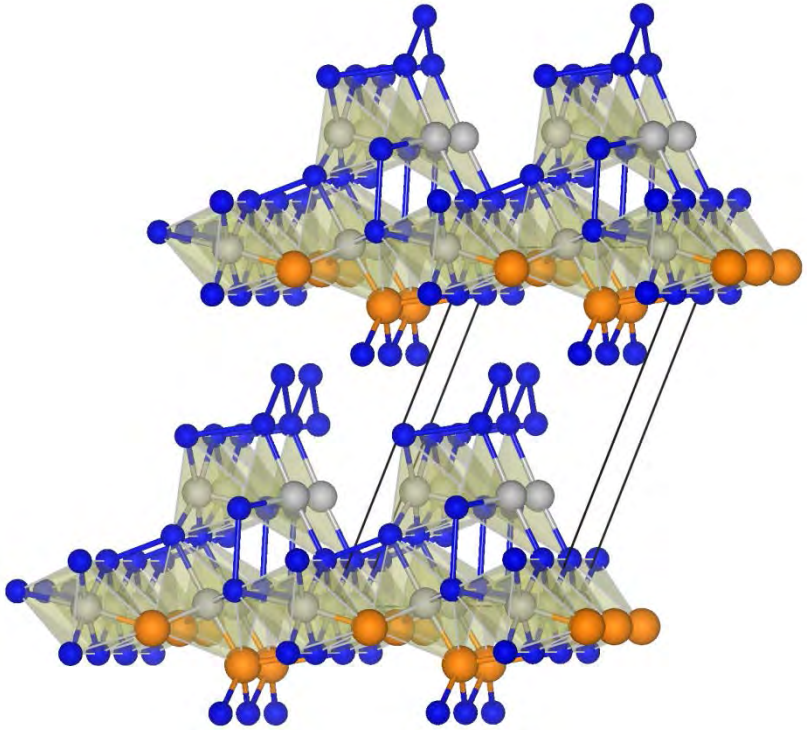
a = 6.78(1) Å, b = 3.30(1) Å, c = 10.75(2) Å

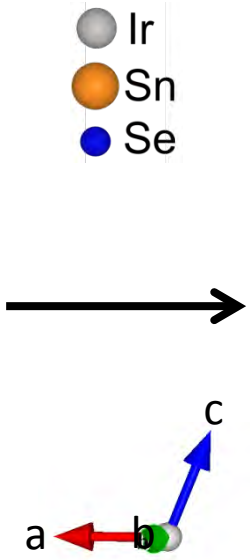
- Then ran Unit Cell search in TOPAS – found several similar to

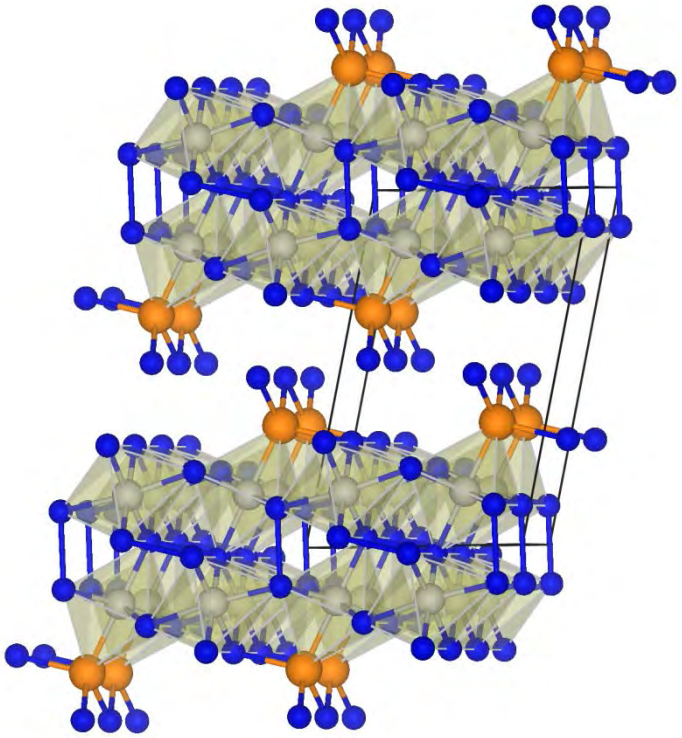
$P2/m$ (10) a = 7.66 Å, b = 3.75 Å, c = 13.2 Å, γ = 112.4°

within 10% error!

Ir-Sn-Se Simulated Annealing+







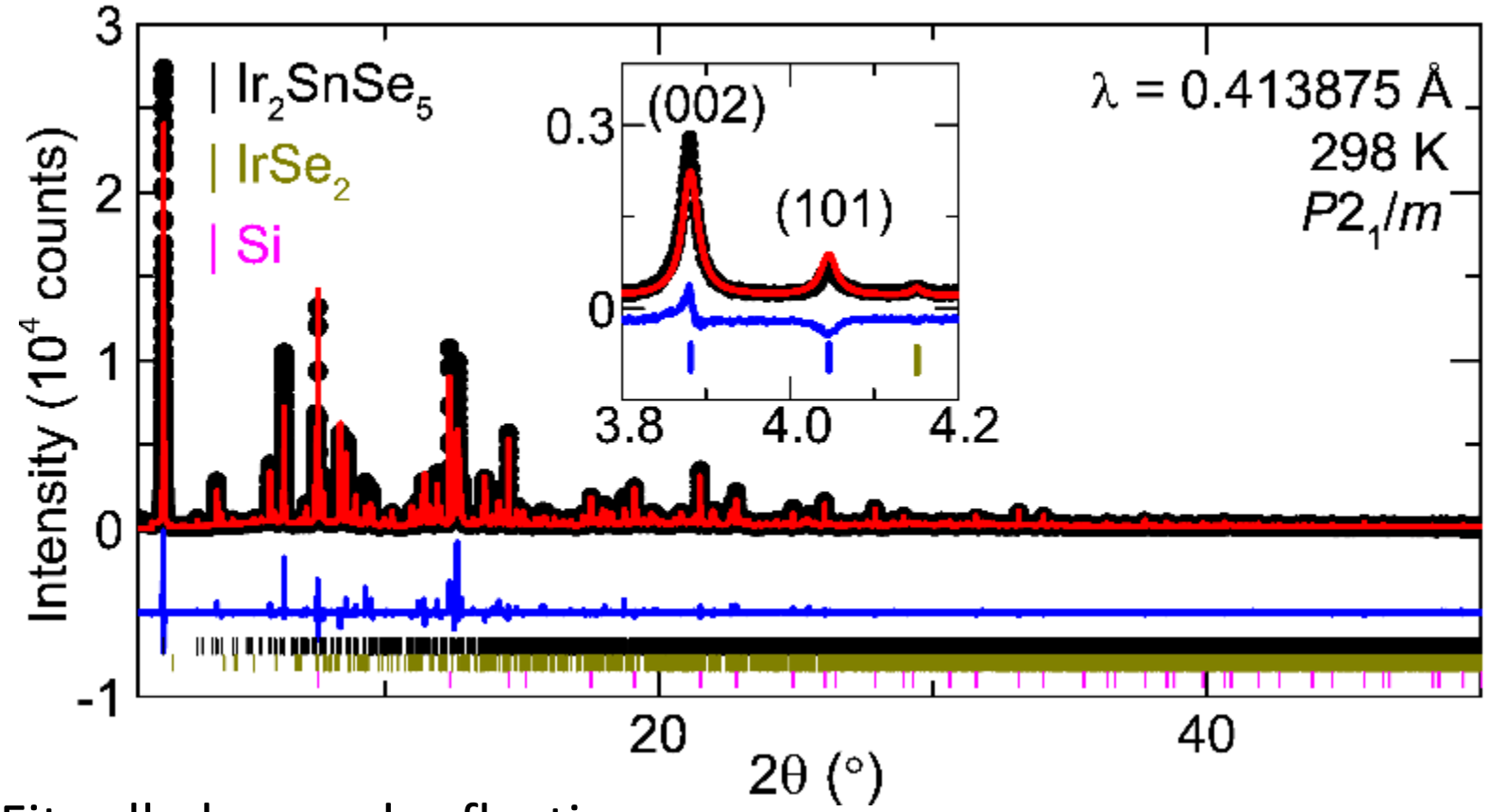
- SA Yielded: *P*1 (1)

a = 7.66 Å, *b* = 3.75 Å,
c = 13.2 Å, γ = 112.4°

- Fixed Model: *P*2/m (10)

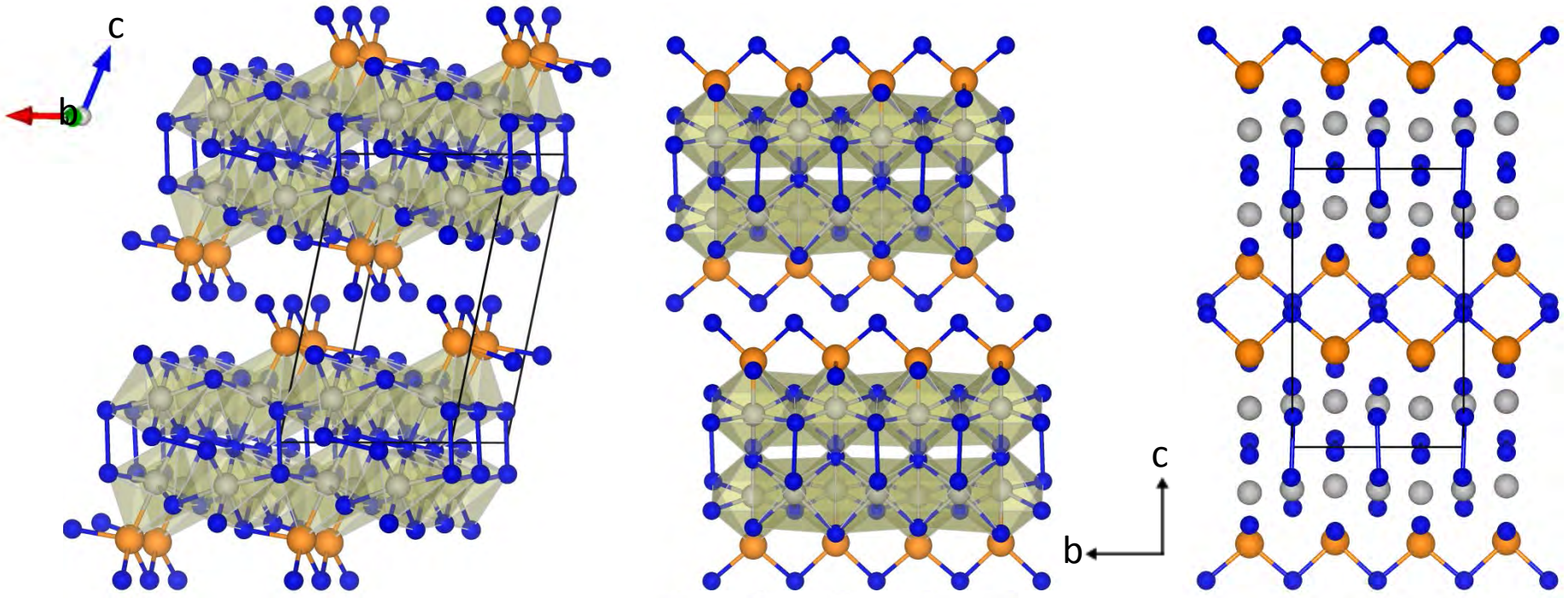
a = 7.66 Å, *b* = 3.75 Å,
c = 12.5 Å, γ = 102.08°
Formula $(IrSe_2)_2SnSe$!

Refinement of Ir_2SnSe_5



- Fits all observed reflections
- 1.75 wt% $IrSe_2$ impurity present
- Hamilton R-ratio test denies lower symmetry spacegroups with 99.99% certainty (Hamilton, W.C. *Acta Cryst*. **18** 502 (1965).)

Ir_2SnSe_5 Structure

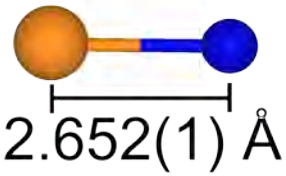


- Similar to $IrSe_2$ – but with SnSe polymeric chain "capping" each layer

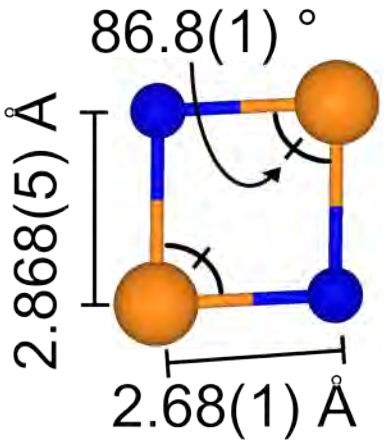
- Formally: $Ir^{3+}{}_2(Se_2)^{2-}Se^{2-}{}_2Sn^{2+}Se^{2-}$

Anion-Anion Bonding

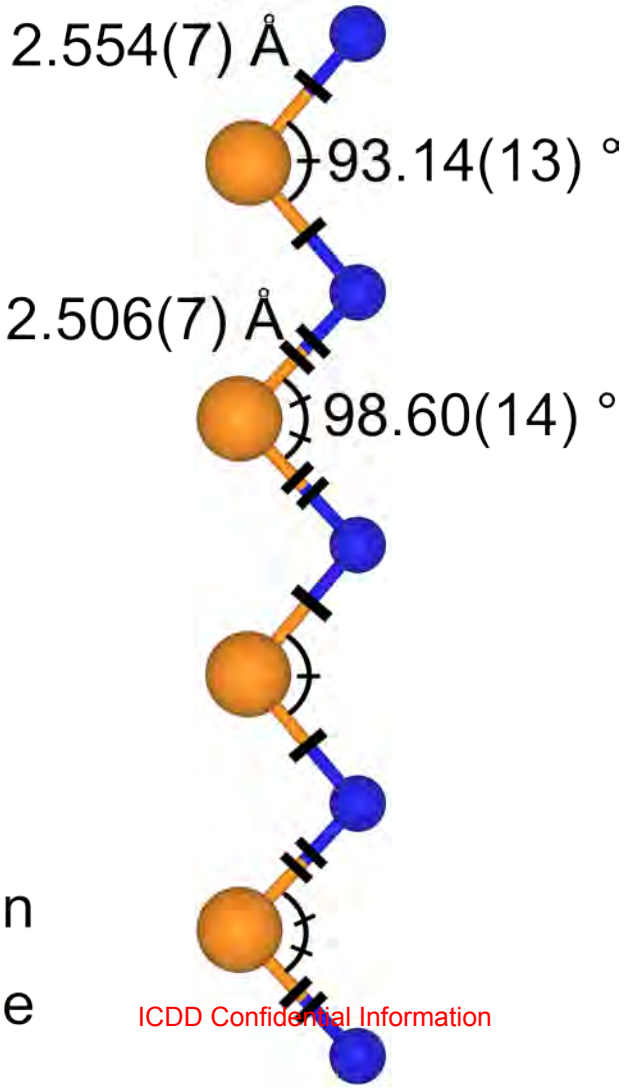
$Ir^{3+}_2(SnSe)^{4-}(Se_2)^{2-}$



$Ir^{3+}_4(Sn_2Se_2)^{4-}_3$



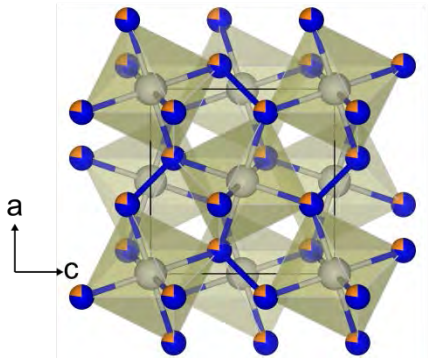
$Ir^{3+}_2(Se_2)^{2-}Se^{2-}_2(SnSe)^{0}$

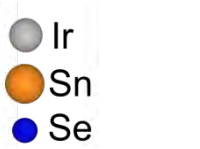


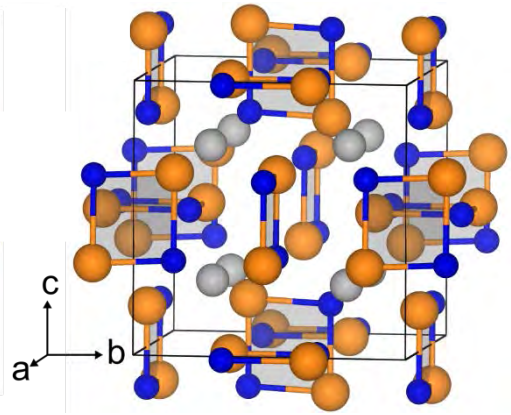
- Each compound has varying degrees of anion-anion bonding
- $IrSn_{0.45}Se_{1.55}$ has monomer
- $Ir_2Sn_3Se_3$ has Sn-Se dimer
- Ir_2SnSe_5 has polymeric chain

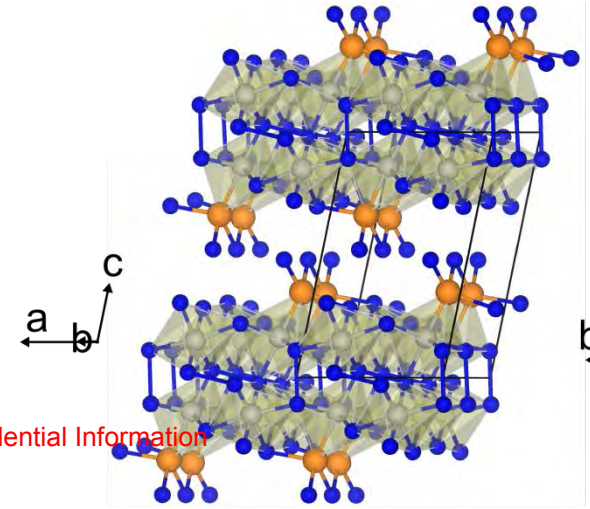
Conclusions

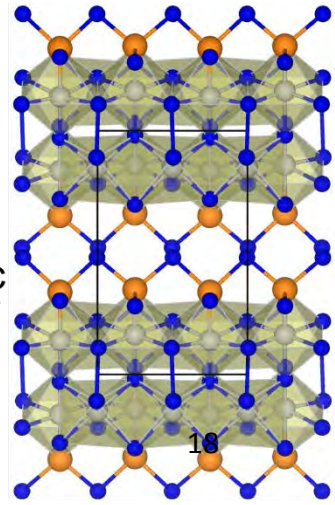
- Pyrite phase $IrSn_{0.45}Se_{1.55}$ has disordered Sn
  - Likely disordered due to Sn only being on every other X-Se monomer
- Skutterudite $Ir_2Sn_3Se_3$ crystallizes in spacegroup $R\bar{3}$ with Sn and Se ordered
- new structure type Ir_2SnSe_5
  - Hamilton R-ration tests confirm spacegroup, Sn position
  - Still Rietveld fit is not great – need to confirm stacking fault











Acknowledgements

Thanks to:

Dr. Allyson M. Fry
Dr. W. Adam Phelan
Dr. Kenneth JT Livi

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NSF Division of Materials Research
Solid Sate Materials and Chemistry
CAREER grant NSF
DMR-1253562

Ludo Frevel Crystallography Scholarship (2014)

PI:
Dr. Tyrel M. McQueen
Department of Chemistry
Department of Physics and Astronomy
Institute for Quantum Matter
http://occamy.chemistry.jhu.edu

Programs:
VESTA
TOPAS
GSAS
SingleCrystal
ICSD Database
ICDD Database
PLATON
Bilbao Crystallographic Server

China

Mianyang Changhong International Hotel

Twelfth National Congress and ICDD Seminar

Year 2015 October 26 to 29

Sponsors

- Chinese Physical Society of Professional Committee of the X-ray diffraction
- China Crystal Society of Professional Committee of Powder Diffraction
- National Natural Science Foundation of China Engineering and Materials Science Department
- China Academy of Engineering Physics
- Beijing Ceramic Society
- Institute of Physics
- *International Centre for Diffraction Data, USA*

ICDD Spring Meetings, Newtown Square, PA, 24 March 2015

Reports of Regional Co-chair, Eastern Pacific Rim

(Japan, Korea & Philippines)

Takashi IDA, Japan

井田　隆（日本）

Advanced Ceramics Research Center,

Nagoya Institute of Technology, Japan

Aichi Synchrotron Radiation Center, Japan

Contents

International Scientific Meetings in Japan & Korea

2014-2015 (8 meetings)

2015-2016 (5 meetings)

Rietveld Refinement as Maximum Likelihood Estimation with a 2D X-ray Detector

Least-squares and maximum likelihood methods

Application of two-dimensional pixel detector to PXRD

International Meetings 2014-2015 (1/8 - 2/8)

1. ICSS-Silicide2014

International Conference and Summer School on Advanced Silicide Technology 2014

Jul. 19 - 21, 2014, Tokyo, Japan

http://annex.jsap.or.jp/silicides/icss-silicide2014/

2. IUMRS-ICA 2014

International Union of Materials Research Societies - International Conference in Asia 2014

Aug. 24 - 30, 2014, Fukuoka, Japan

http://www.Iumrs-Ica2014.org

International Meetings 2014-2015 (3/8 - 4/8)

3. ICTMC-19

19th International Conference on Ternary and Multinary Compounds

Sep. 1 - 5, 2014, Niigata, Japan

http://annex.jsap.or.jp/tmc/ictmc19/index.html

4. WFF - IAFS 2014

World Forensic Festival - 20th World Meeting of the International Association of Forensic Sciences

Oct. 12 - 18, 2014, Seoul, Korea

http://www.wff2014korea.org

International Meetings 2014-2015 (5/8 - 6/8)

5. ICMCB2015

International Conference on Molecular Chemistry and Biochemistry

May 30 - 31, 2015, Narita, Japan

https://www.waset.org/conference/2015/05/tokyo/ICMCB

6. ZMPC2015

International Symposium on Zeolite and Microporous Crystals

2015, Jun. 28 - Jul. 2, 2015, Sapporo, Japan

http://www.knt.co.jp/ec/2015/zmpc/index.html

International Meetings 2014-2015 (7/8 - 8/8)

7. ICCCI 2015

International Conference on the Characterization and Control of Interfaces for High Quality Advanced Materials and the 51st Summer Symposium on Powder Technology

Jul. 7 - 10, 2015, Kurashiki, Japan

http://ceramics.ynu.ac.jp/iccci2015/index.html

8. ICSAM2015

12th International Conference on Superplasticity in Advanced Materials 2015

Sep. 7 - 11, 2015, Tokyo, Japan

http://icsam2015.jp Abstract deadline: Feb. 1

International Meetings 2015-2016 (1/5 - 2/5)

1. ICCOSS XXII

The 22nd International Conference on the Chemistry of the Organic Solid State

Jul. 12 - 17, 2015, Niigata, Japan

http://www.iccoss2015.org

Abstract deadline: Mar. 26

Support of ICDD for young scientists' participation ?

Local Chair: Prof. Uekusa

2. IUPAC-2015

International Union of Pure and Applied Chemistry, 48th General Assembly & 45th World Chemistry Congress

Aug. 6 - 14, 2015, Busan, Korea

http://www.iupac2015.org

Abstract deadline: Apr. 30

International Meetings 2015-2016 (3/5 - 4/5)

3. APT 2015

The 6th Asian Particle Technology Symposium

Sep. 15 - 18, 2015, Seoul, Korea

http://apt2015.org Abstract deadline: Mar. 31

4. Crystallization 2015

11th International Symposium on Crystallization in Glasses and Liquids

Oct. 11 - 14, 2015, Nagaoka, Japan

http://crystallization-2015.jp Abstract deadline: Mar. 31

International Meetings 2015-2016 (5/5)

5. IUMRS-ICAM 2015

14th International Union of Materials Research Societies - International Conference on Advanced Materials 2015

Oct. 25 - 29, 2015, Jeju, Korea

http://iumrs-icam2015.org Abstract deadline: May 31

Rietveld Refinement as Maximum Likelihood Estimation with a Two-Dimensional X-ray Detector

Rietveld Refinement as Maximum Likelihood Estimation with a Two-Dimensional X-ray Detector

"Particle statistics in PXRD",
ICDD Spring Meeting 2010.
→ We can measure crystallite size about 5–50 μm

"Analytical method based on maximum likelihood",
ICDD Spring Meeting 2012, DXC 2012.
→ Not least-squares (LSQ), but maximum-likelihood (ML) method should be used ?

"PXRD BL in a small SR facility, AichiSR in Japan",
ICDD Spring Meetings 2013, 2014.
→ Use of 2D-detector ?

Rietveld Refinement as Maximum Likelihood Estimation with a Two-Dimensional X-ray Detector

"Practical statistics in PXRD"

Suggestion on ICDD Spring Meeting 2015:

"The Rietveld method can still be used as a maximum-likelihood estimation, if a 2D X-ray detector is used on a synchrotron powder beam line." (Ida, IUCr2014)

→ 2D-detector on SR-PXRD-BL really works !

→ Use of 2D-detector ?

Rietveld Refinement as Maximum Likelihood Estimation with a Two-Dimensional X-ray Detector

"Particle statistics in PXRD",
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Rietveld Refinement as Maximum Likelihood Estimation with a Two-Dimensional X-ray Detector

"Particle statistics in PXRD",
ICDD Spring Meeting 2010.

ML ~ appropriate weight in LSQ ?

Jim Kaduk

m likeli

ICDD Spring Meeting 2012, DXC 2012.

ikelihood (ML)

Can too many significant digits of lattice constants be reduced by use of ML ?

n Japan",
ICDD Spring Meetings 2013, 2014.

→ Use of 2D-detector ?

Mapping of 2D pixel intensities to (2θ, Intensity) data

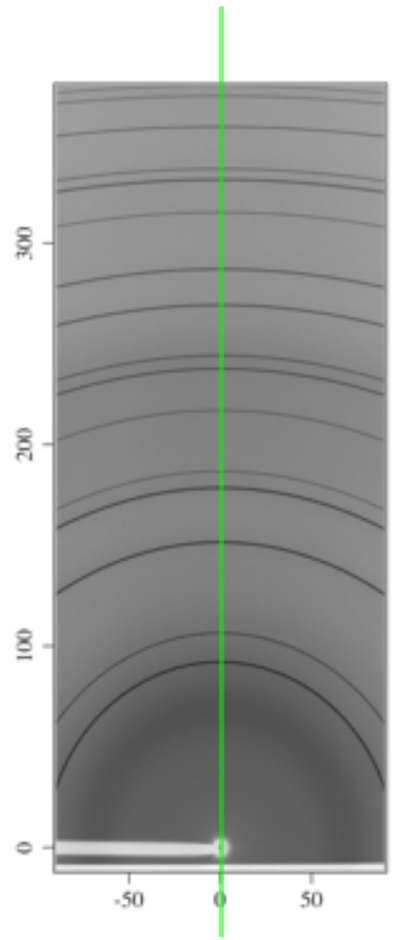
Method of Sulyanov *et al.* (1994)

(= Calculation of average pixel intensity on "meridian")

- uses all live pixel intensities w/o worrying about dead pixels,
- can apply any kind of correction/calibration,
- allows any camera length and 2θ-step,
- will give "aberration-free" data.

Extension of Sulyanov *et al.*'s method

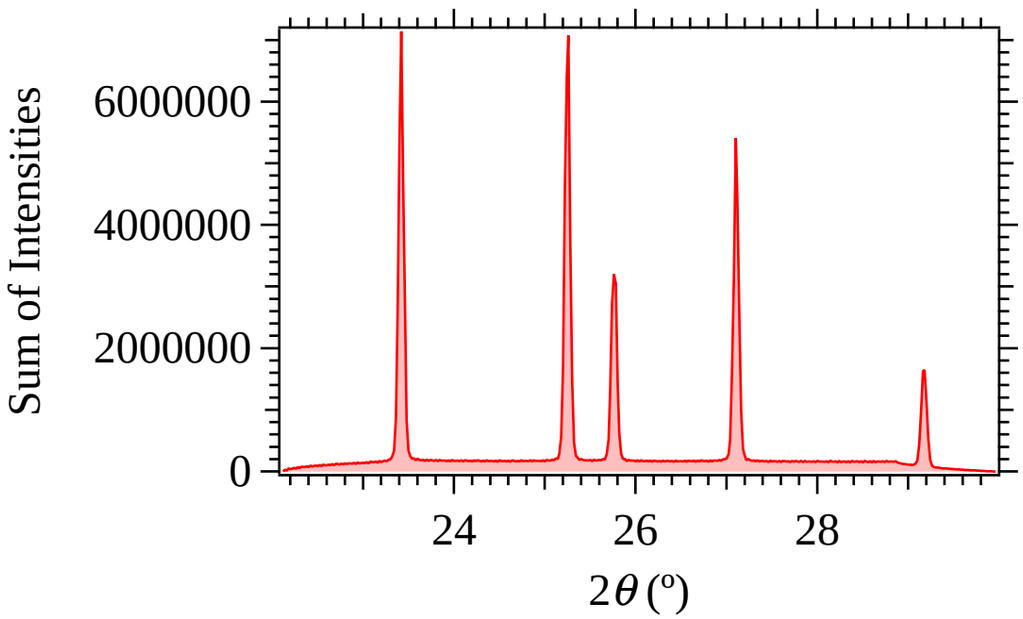
"We can estimate standard deviation of the average intensity".

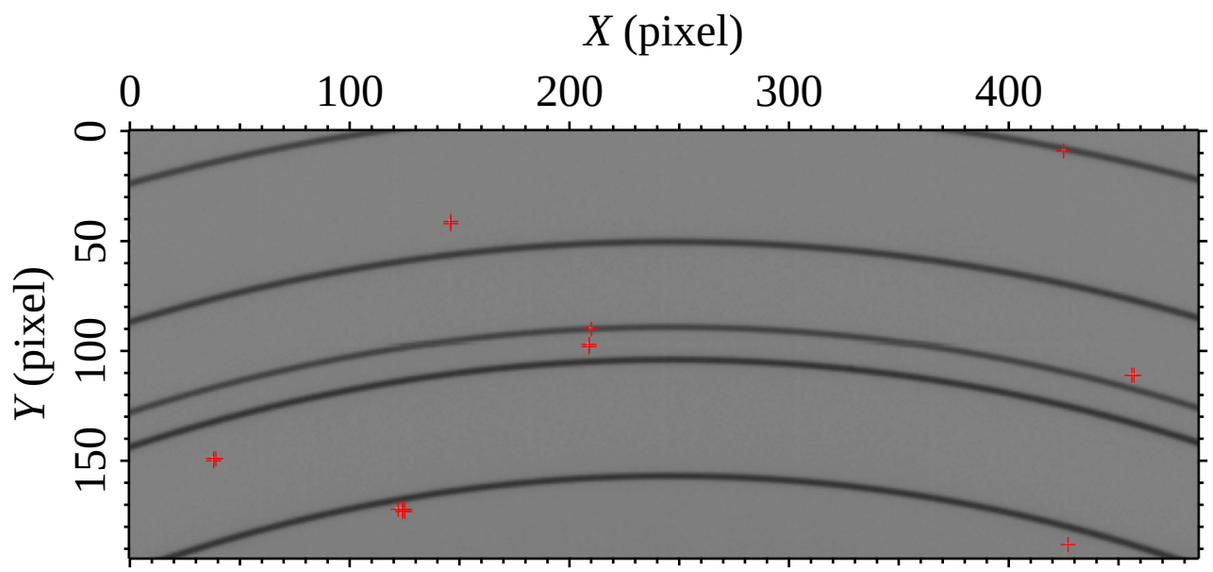


meridian

Experimental and Analysis

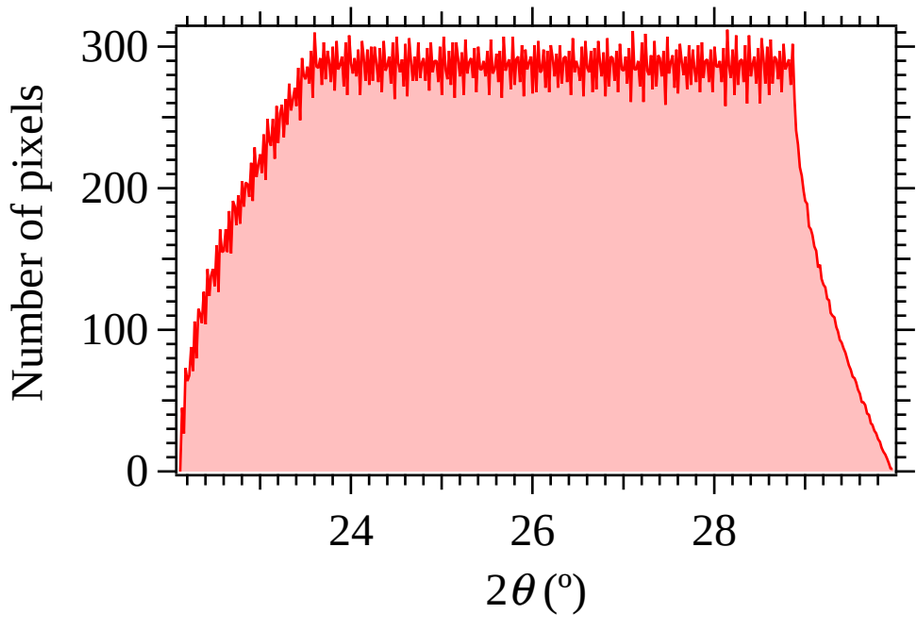
Mapping of data





PILATUS100K, BL5S2@AichiSR

Sum of intensities



Number of pixels

487×195 pixel^2, 0.172 mm/pixel

Peak wavelength: λ = 1.00058 Å

Distance to camera center: R = 284.19 mm

(Resolution at camera center: 0.035°)

Location of camera center: 2Θ = 25.4°

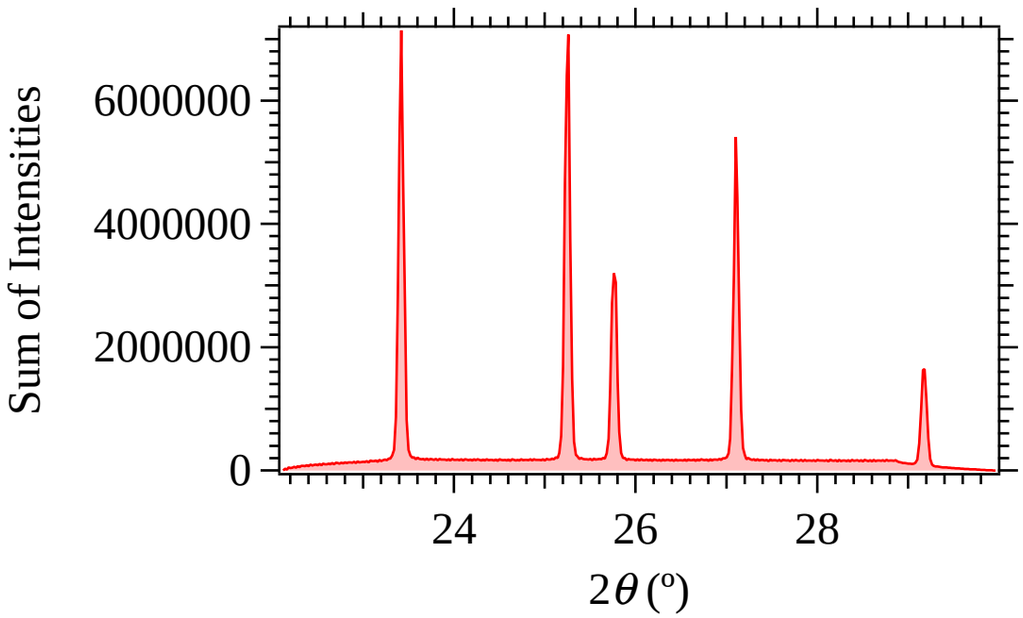
Sample: Quartz (<3 μm) 0.5 mmΦ capillary

Exposure 600 s,

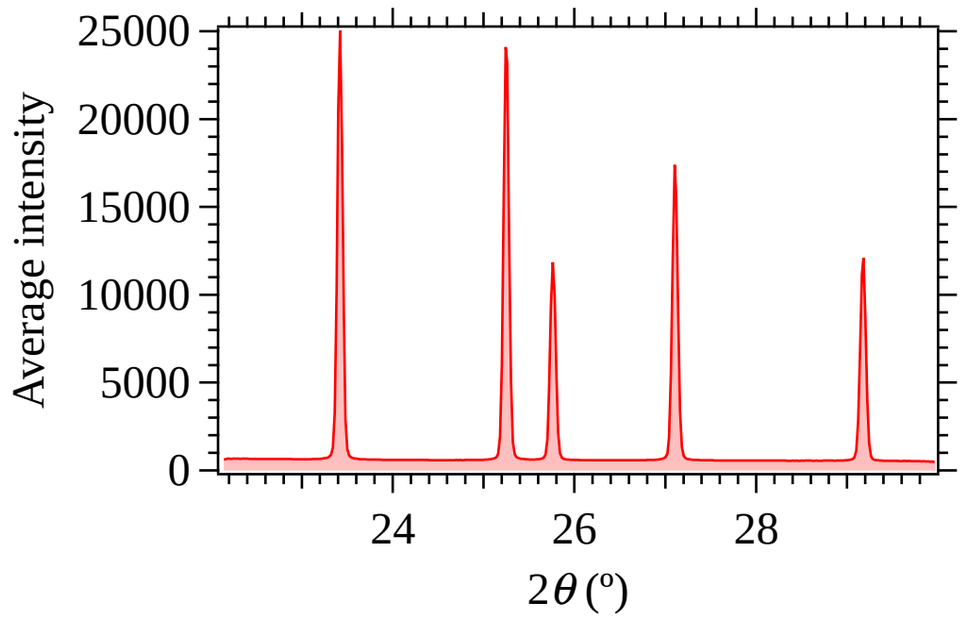
2θ step for mapping: $\Delta 2\theta$ = 0.02°

Experimental and Analysis

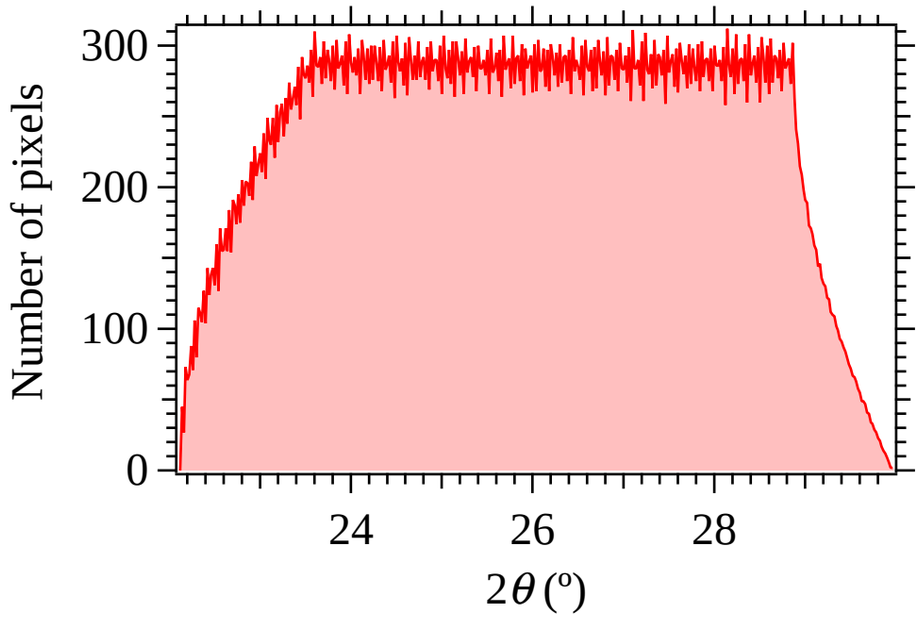
Calculation of average pixel intensities



Sum of intensities



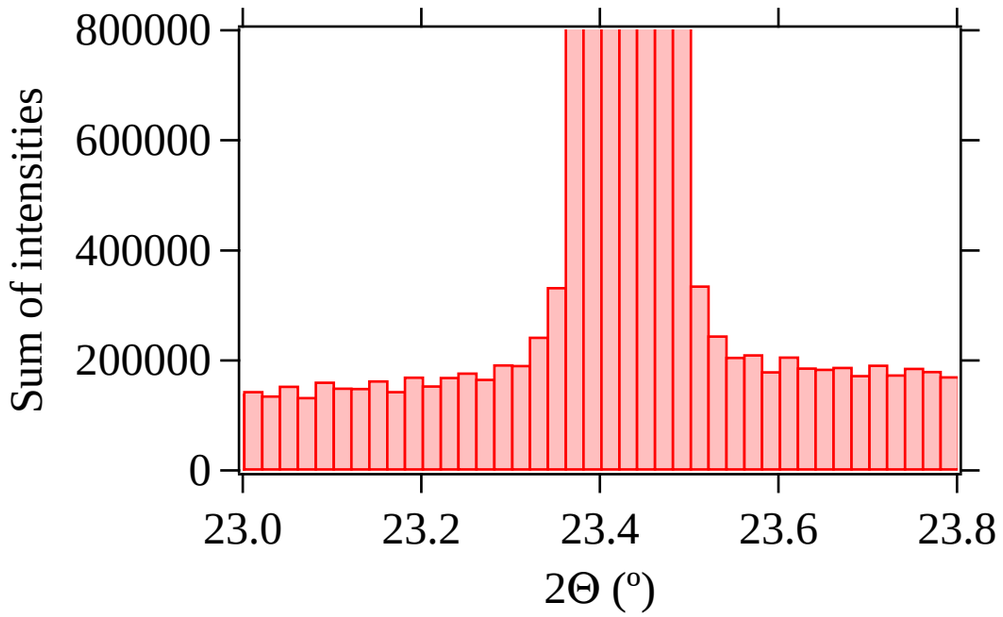
Average intensity



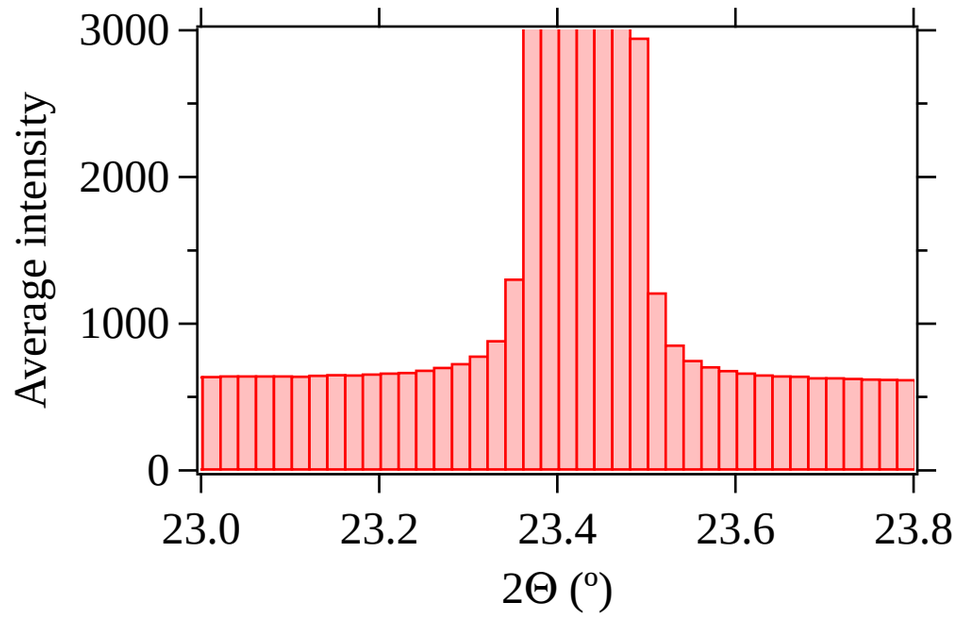
Number of pixels

Experimental and Analysis

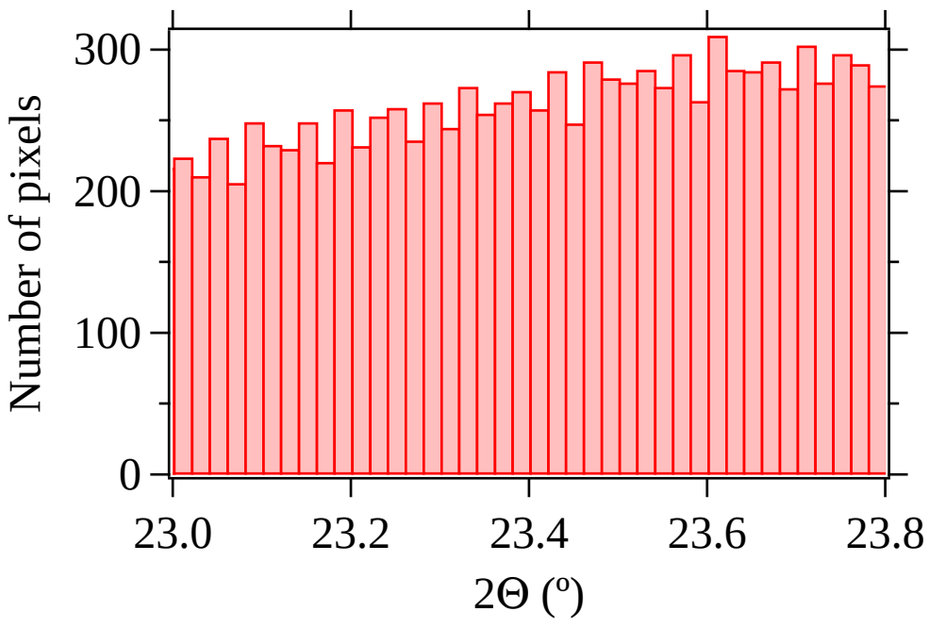
Calculation of average pixel intensities



Sum of intensities



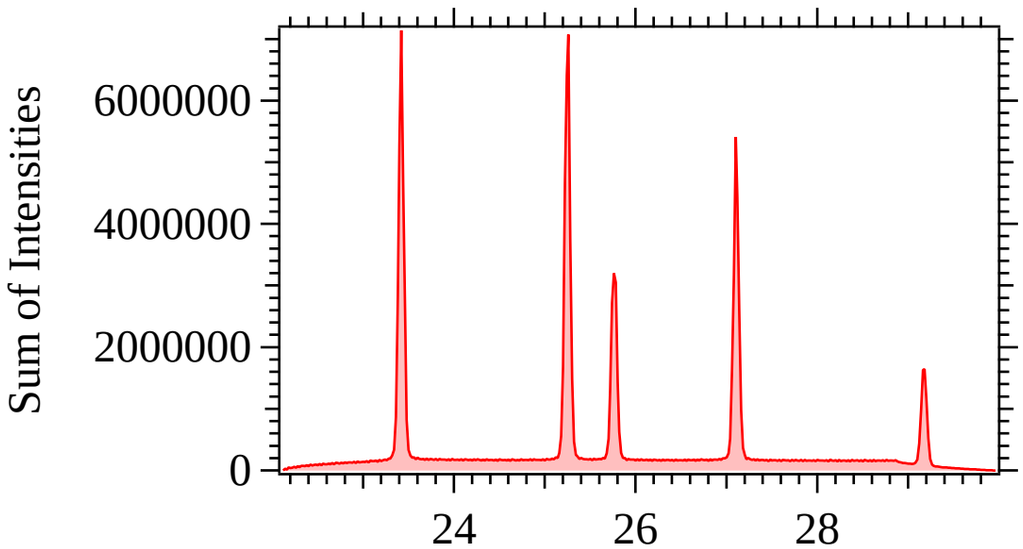
Average intensity



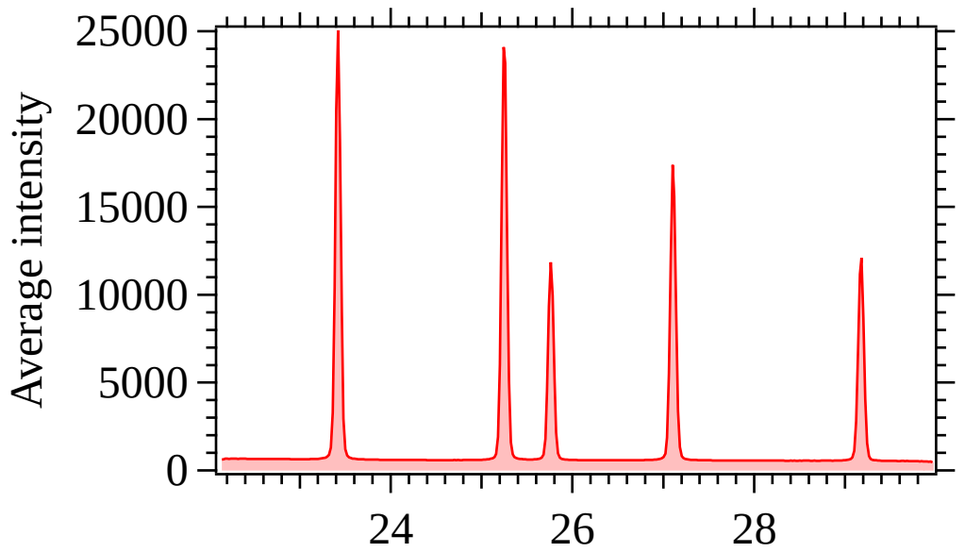
Number of pixels

Experimental and Analysis

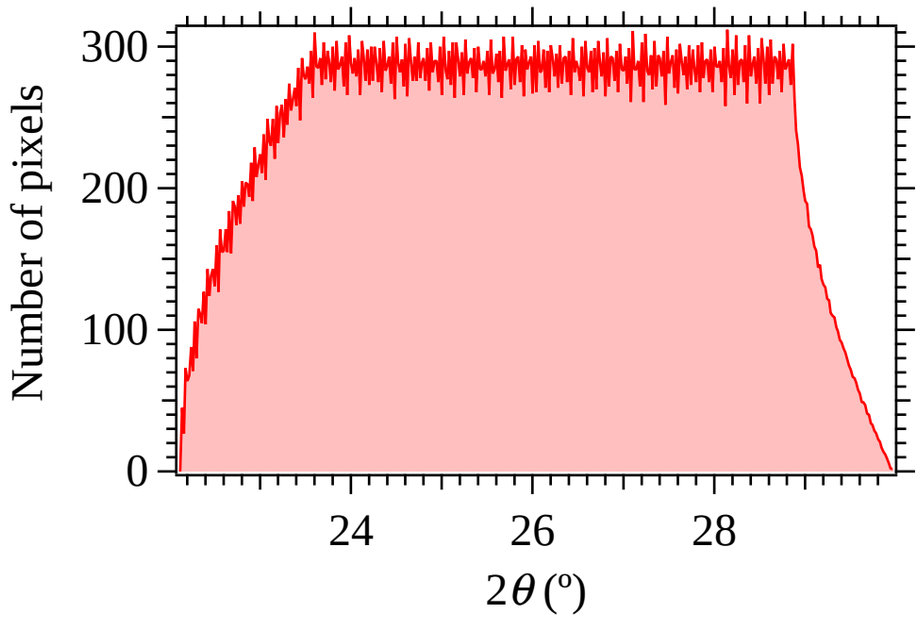
Calculation of average pixel intensities



Sum of intensities



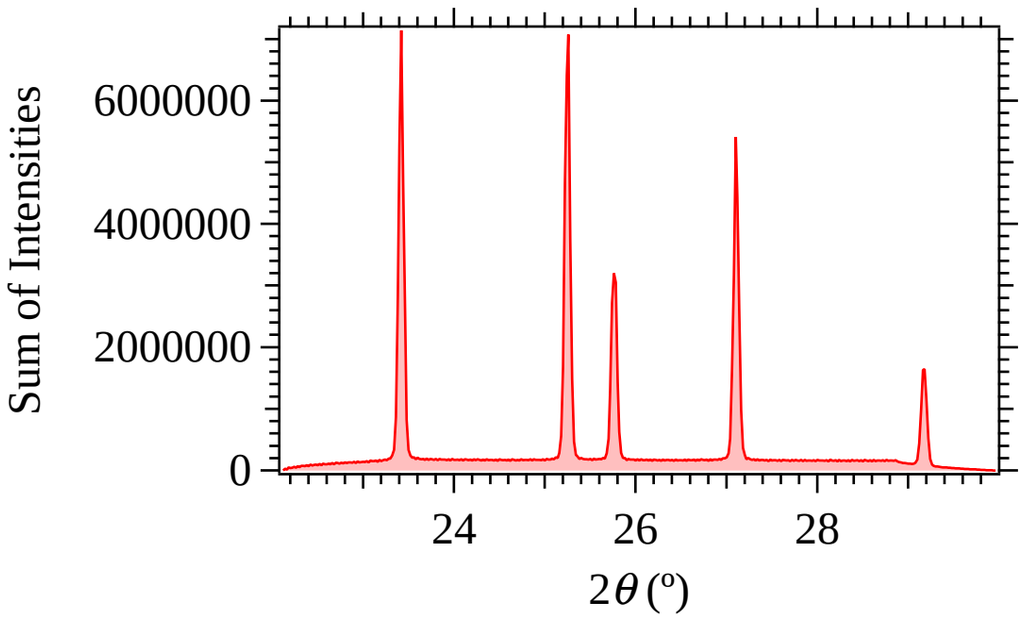
Average intensity



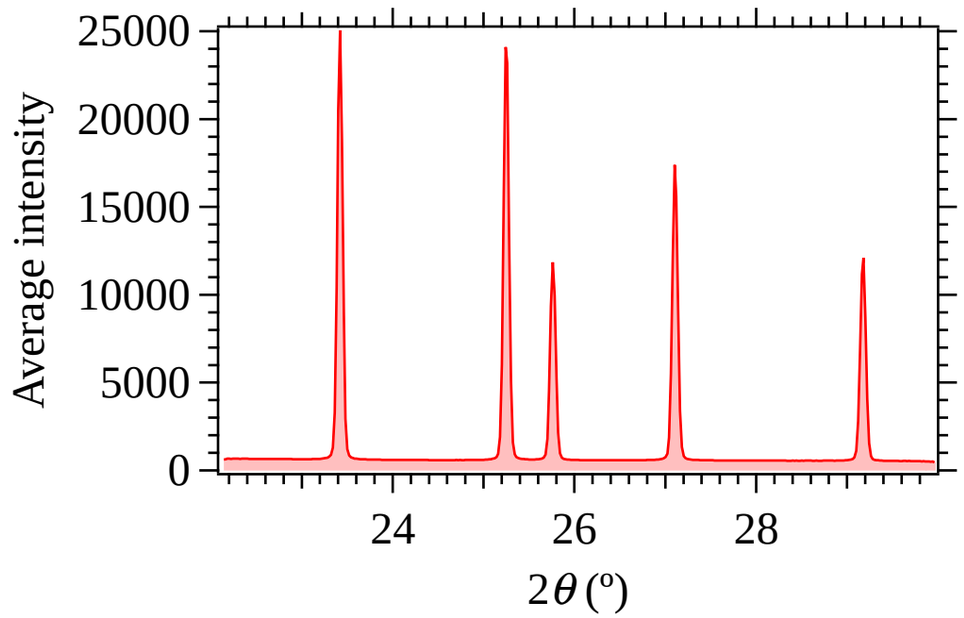
Number of pixels

Experimental and Analysis

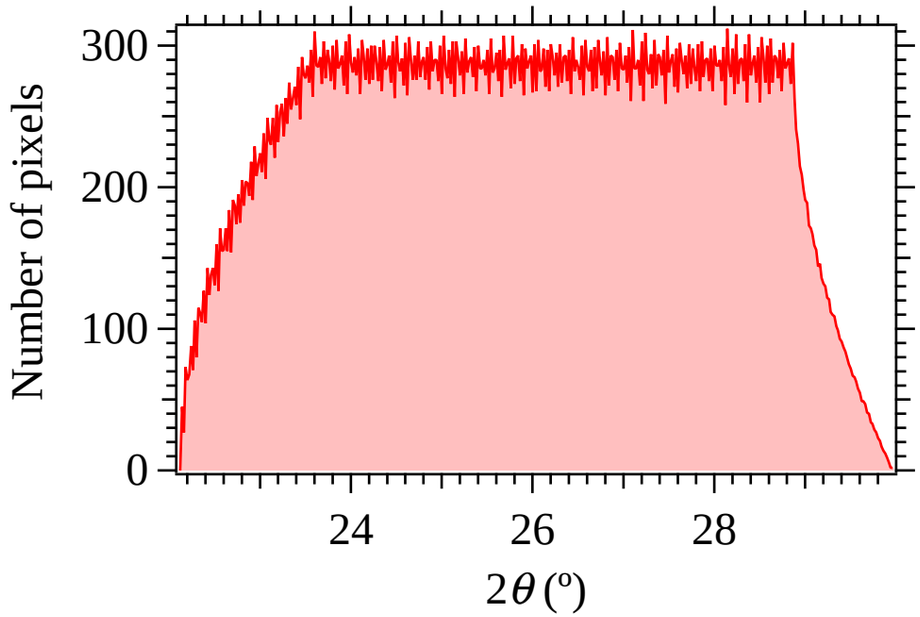
Calculation of average & standard deviation



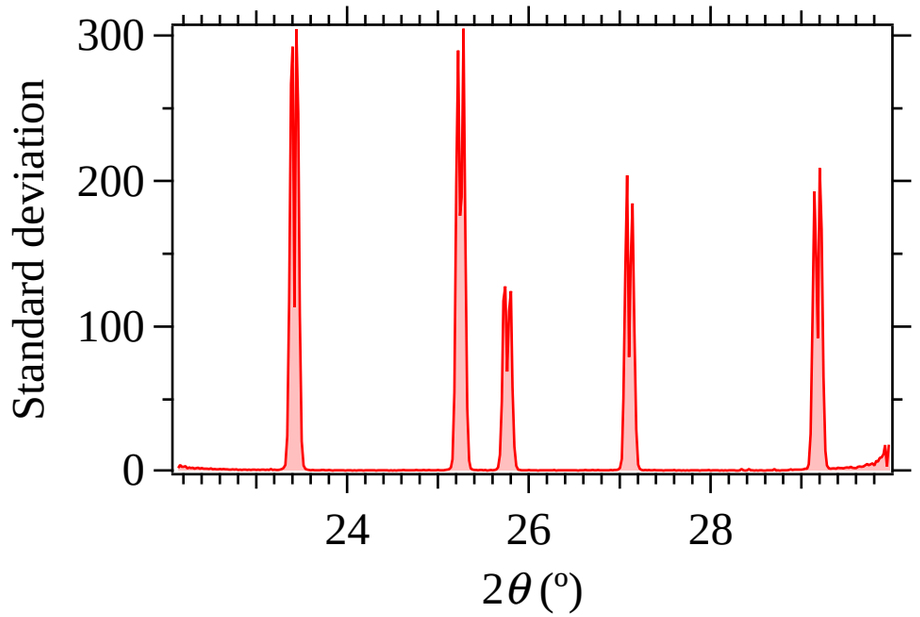
Sum of intensities



Average intensity



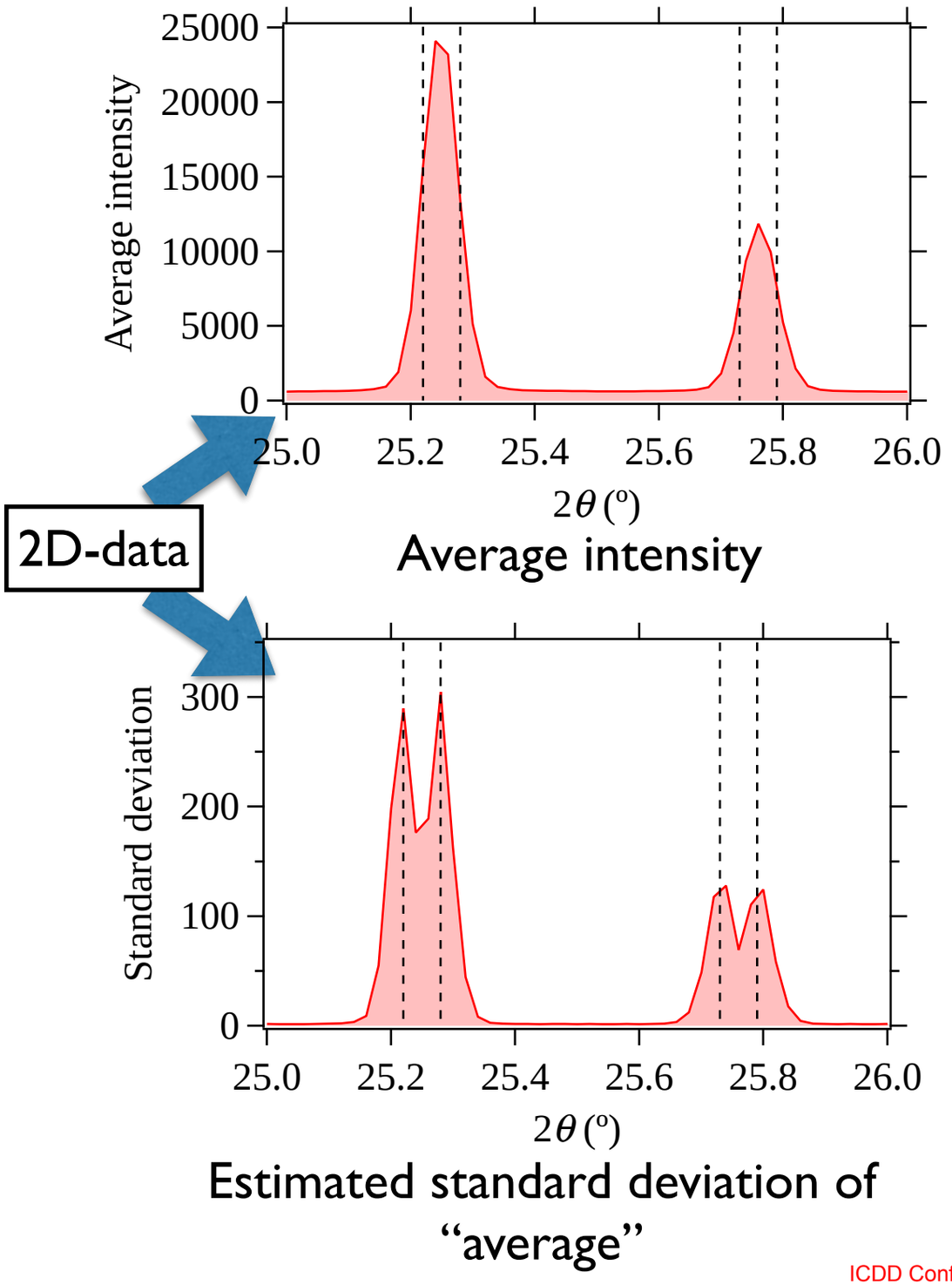
Number of pixels



Standard deviation of "average"

Experimental and Analysis

Calculation of average & standard deviation

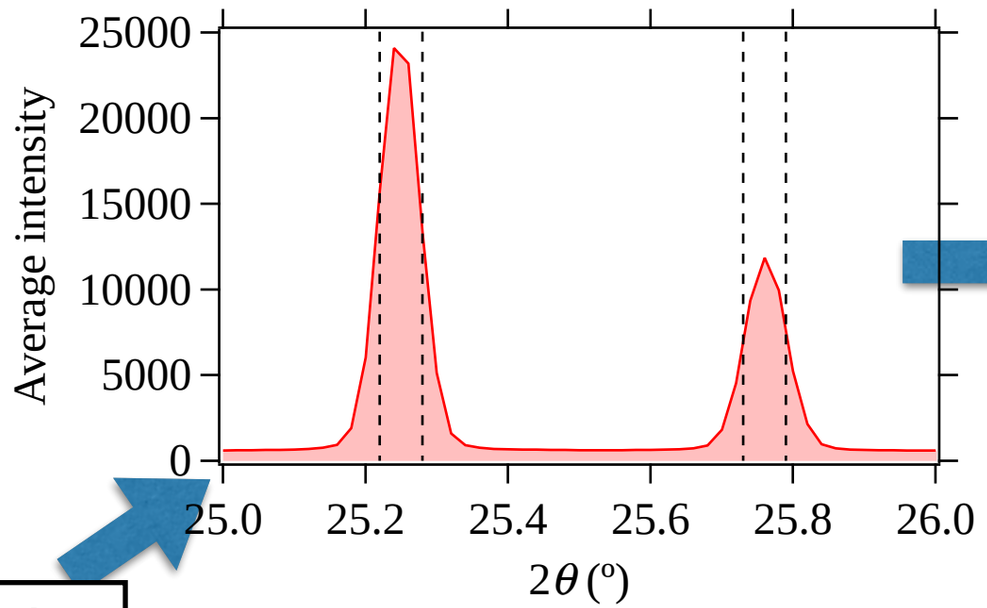


Average intensity

Estimated standard deviation of "average"

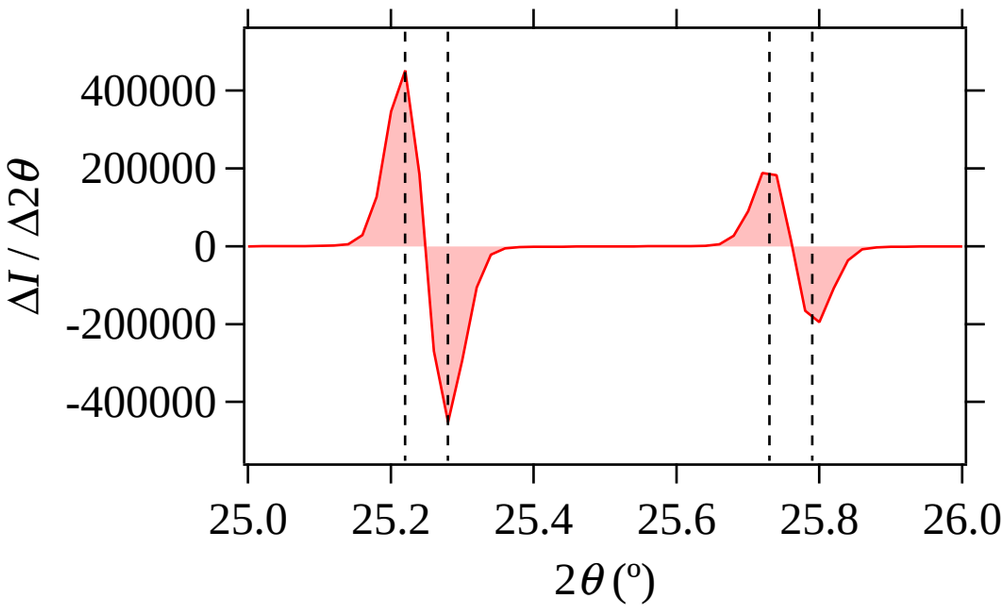
Experimental and Analysis

Calculation of average & standard deviation

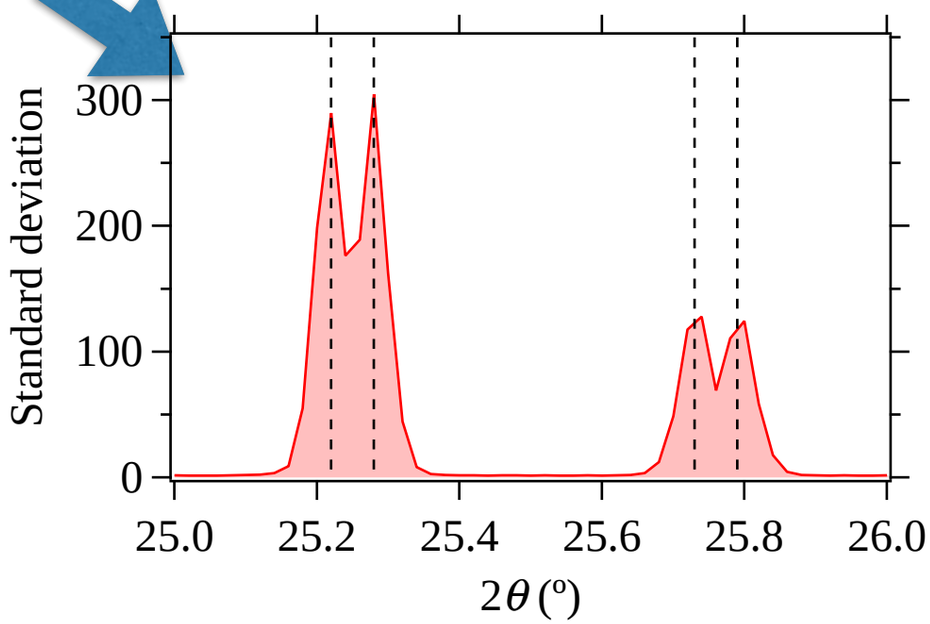


2D-data

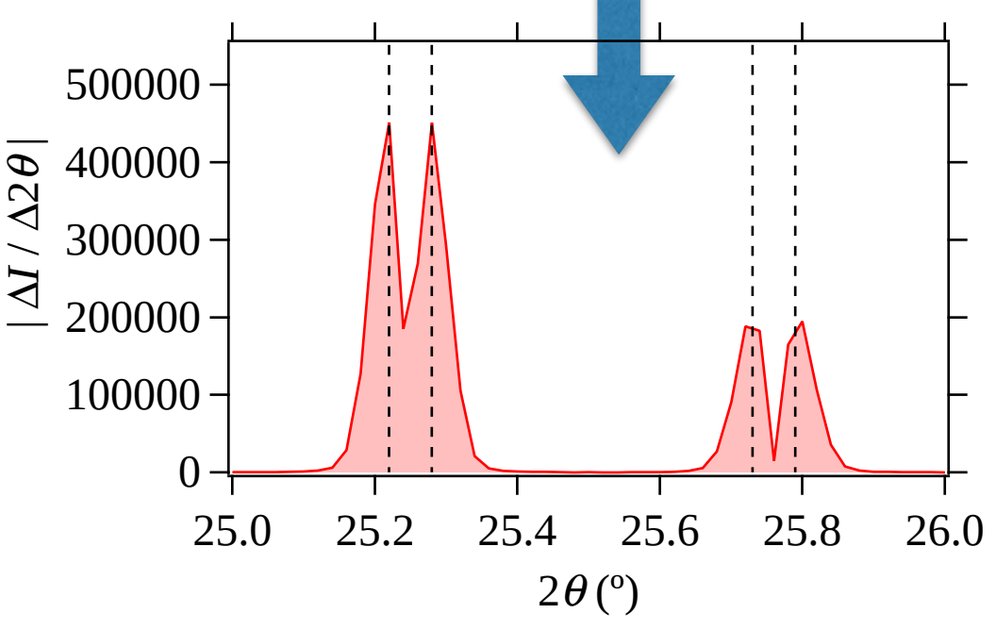
Average intensity



Differential of "average" intensity



Estimated standard deviation of "average"

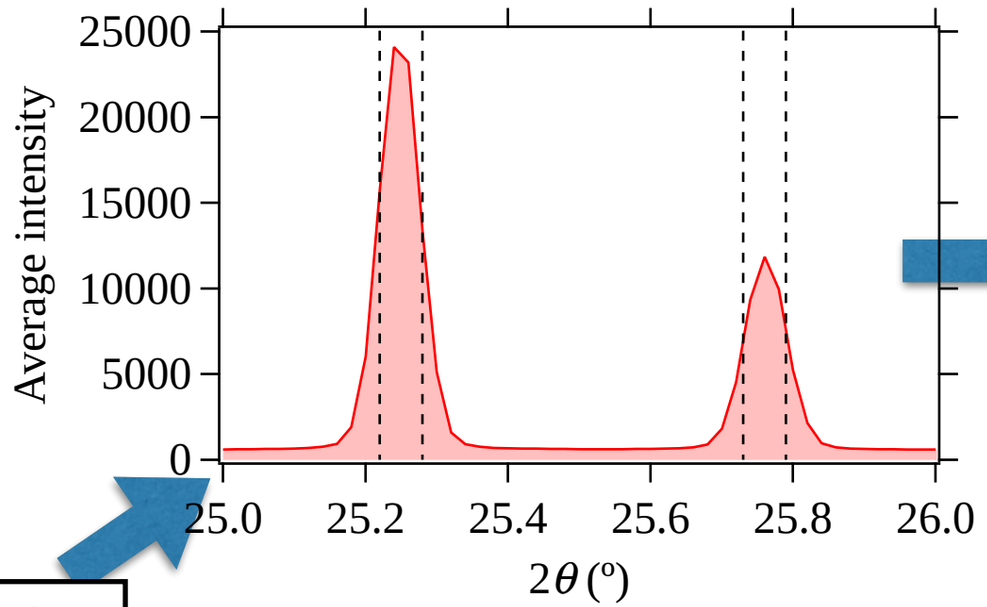


Absolute value of differential

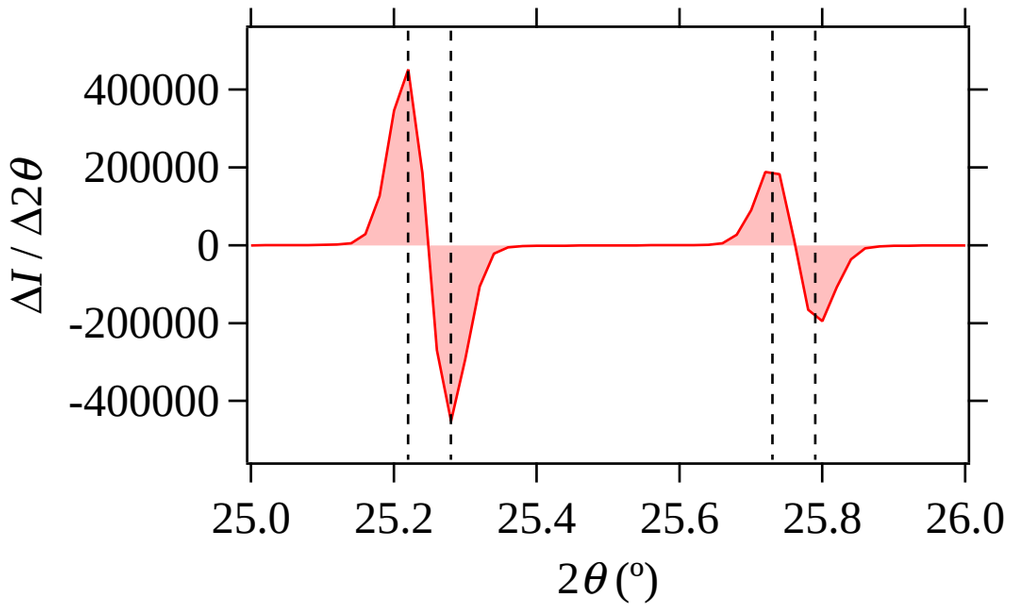
Experimental and Analysis

Calculation of average & standard deviation

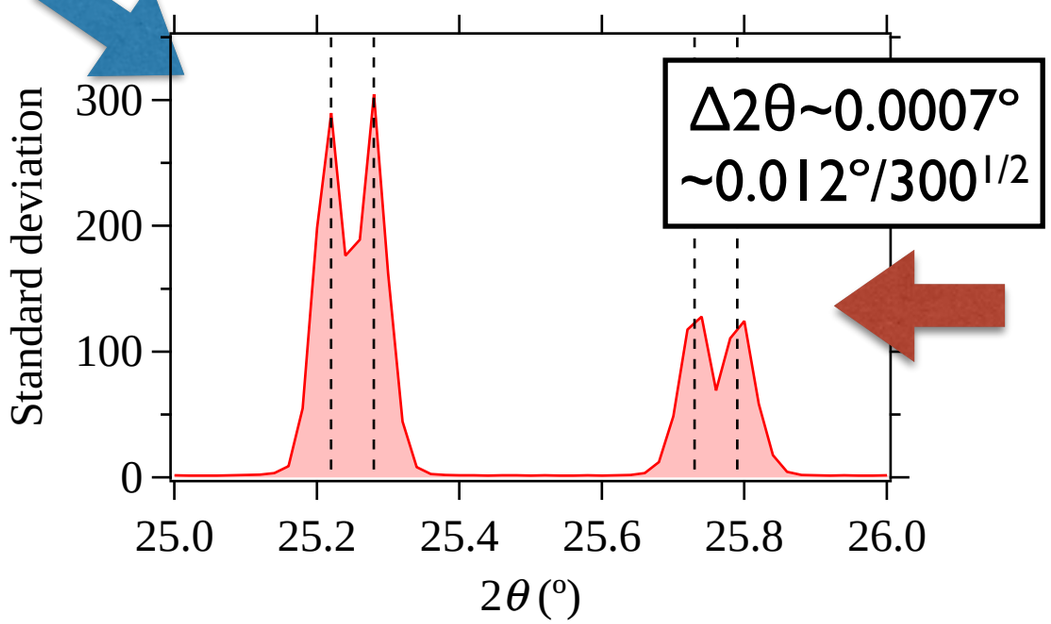
2D-data



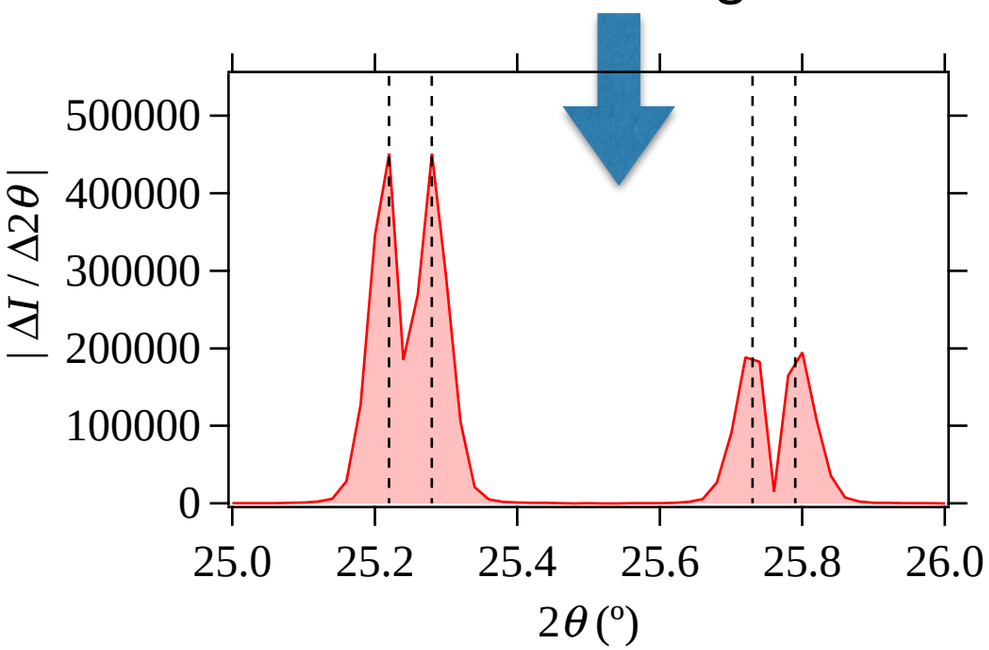
Average intensity



Differential of "average" intensity



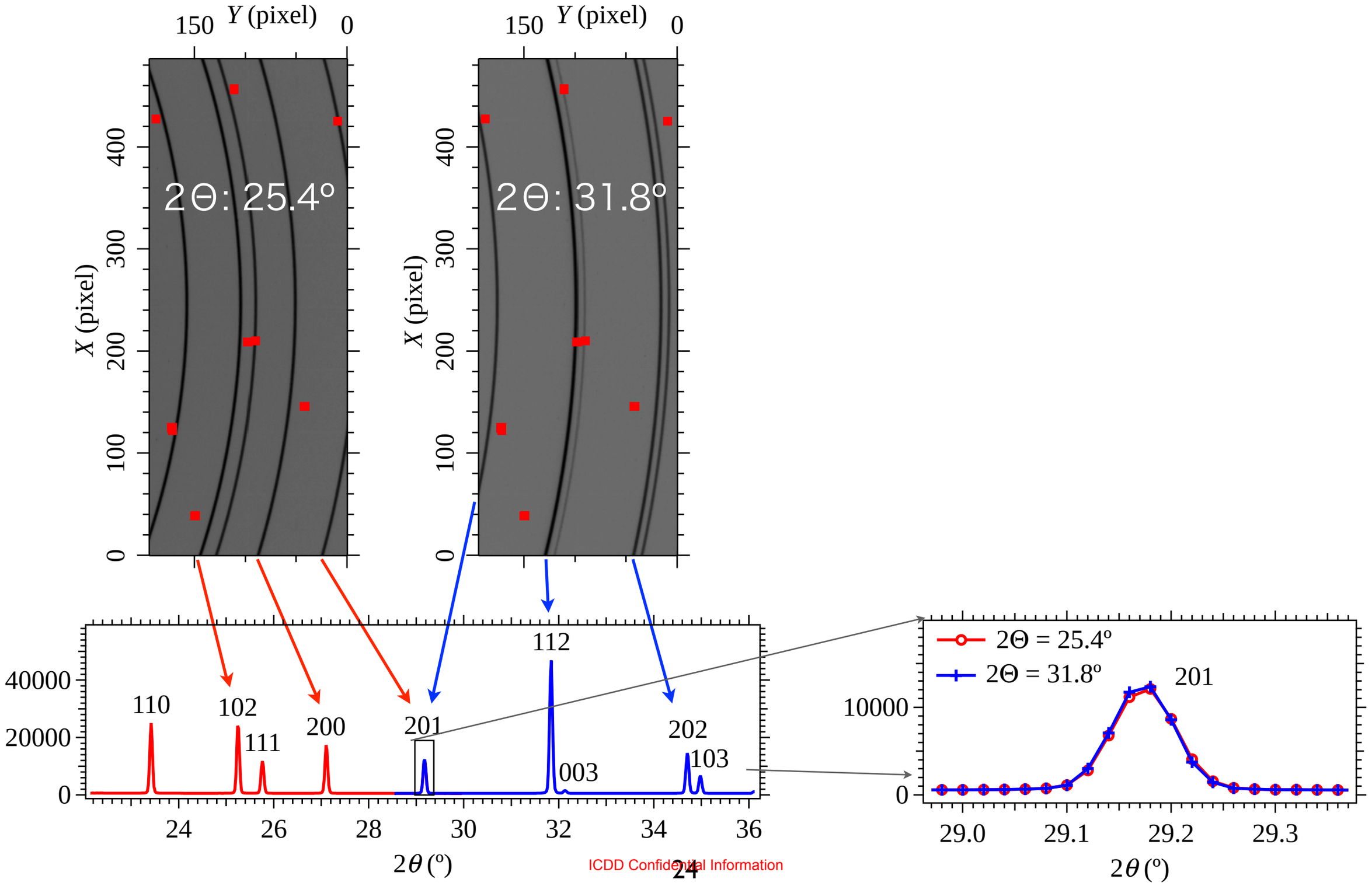
Estimated standard deviation of "average"



Absolute value of differential

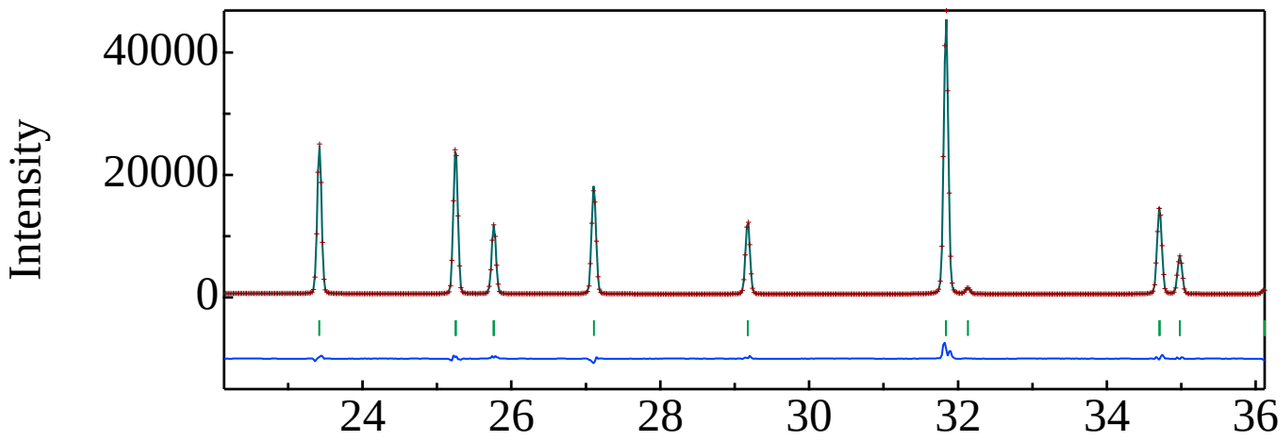
Experimental and Analysis

Connection of segmented data



Experimental and Analysis

Weighted least-squares analysis



Error	(Intensity)$^{1/2}$	Observed
R_{wP} (%)	2.81	0.86
R_P (%)	1.88	2.93
R_B (%)	3.14	3.61
S	1.08	2.98
a (Å)	4.93026(9)	4.9307(4)
c (Å)	5.42342(6)	5.4236(2)

RIETAN-FP (Izumi & Momma, 2007)

profile: symmetric pseudo-Voigt function

peak-shift : constant peak shift

peak-width : Caglioti *et al.* (1958)

background : 11-order polynomials

quartz, trigonal, $P3_121$ (S.G. #152)

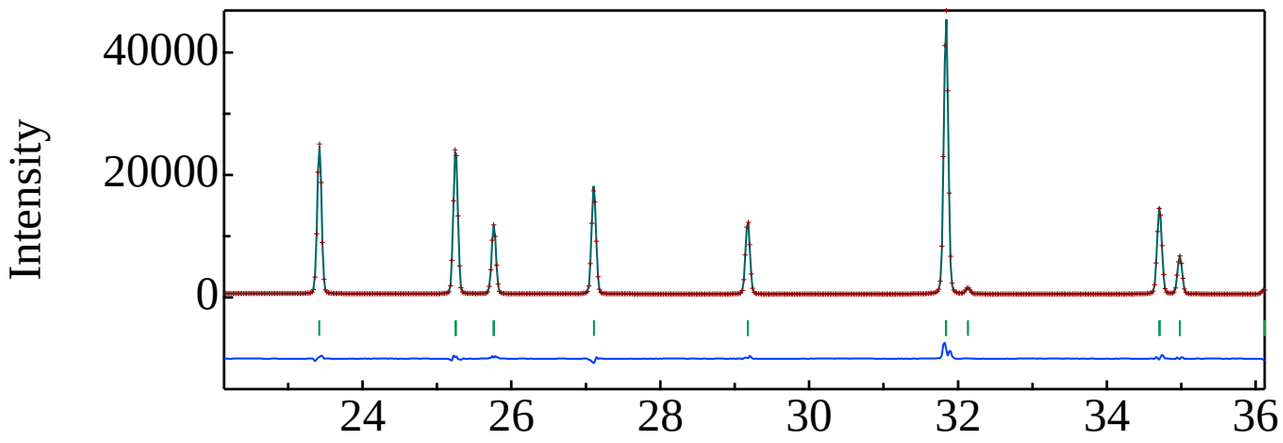
atomic scattering factor : neutral atom

dispersion : Cromer & Liberman (1981)

displacement factor: isotropic

Experimental and Analysis

Weighted least-squares analysis



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S	1.08	2.98
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c (Å)	5.42342(6)	5.4236(2)

TOO MUCH !!!

Modest, but errors still a little underestimated

Rietveld Refinement as Maximum Likelihood

E… X-ray

D…

Can too many significant digits in lattice constants be reduced by use of ML ?

ICDD Spring Meeting 2010.

ML ~ appropriate weight in LSQ ?

5–50 μ…

…m likeli…

Jim Kaduk

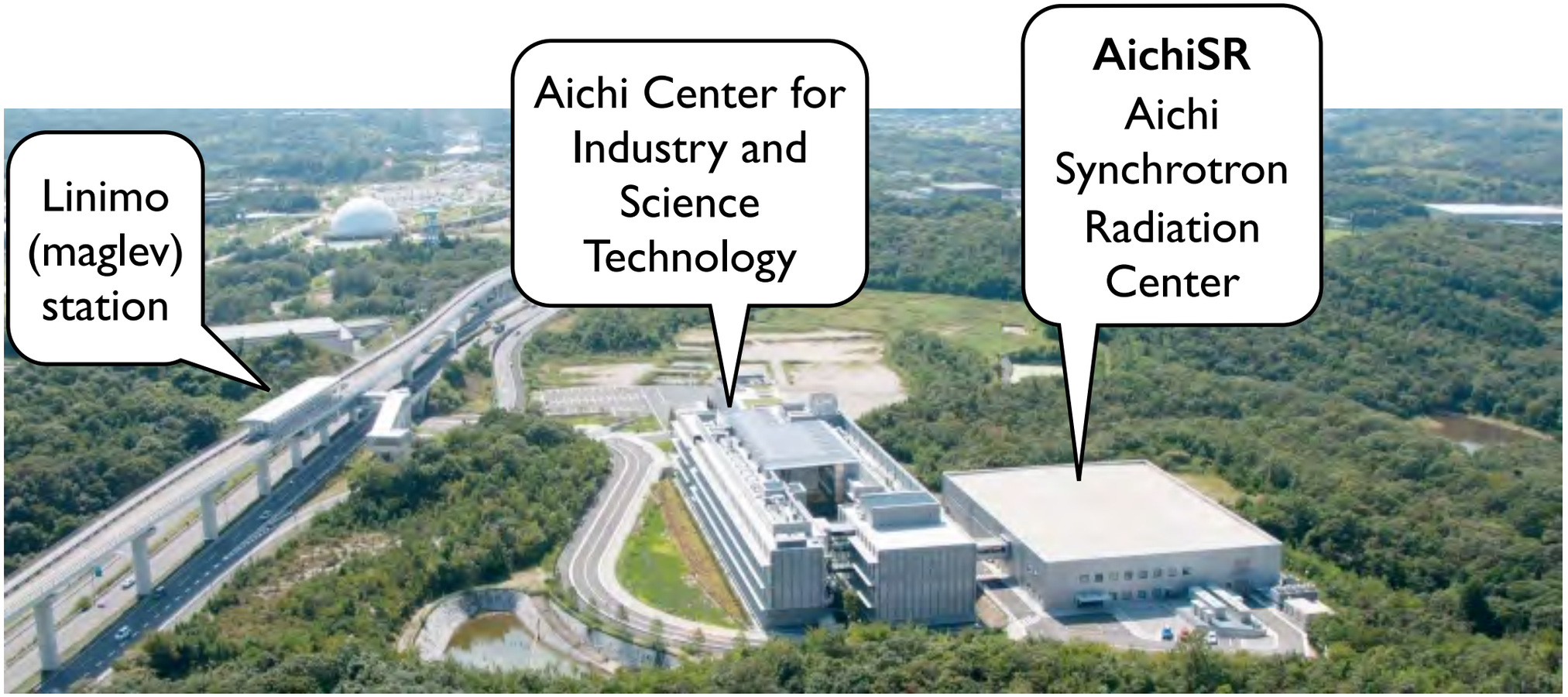
ICDD Spring Me…g 2012, DXC 2012.

…um-likelihood (ML)

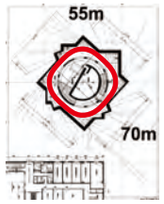
"Appropriate-weight LSQ = ML" can be achieved by 2D-PXRD. Significant digits of LC has approached to reasonable numbers

…SR in Japan",

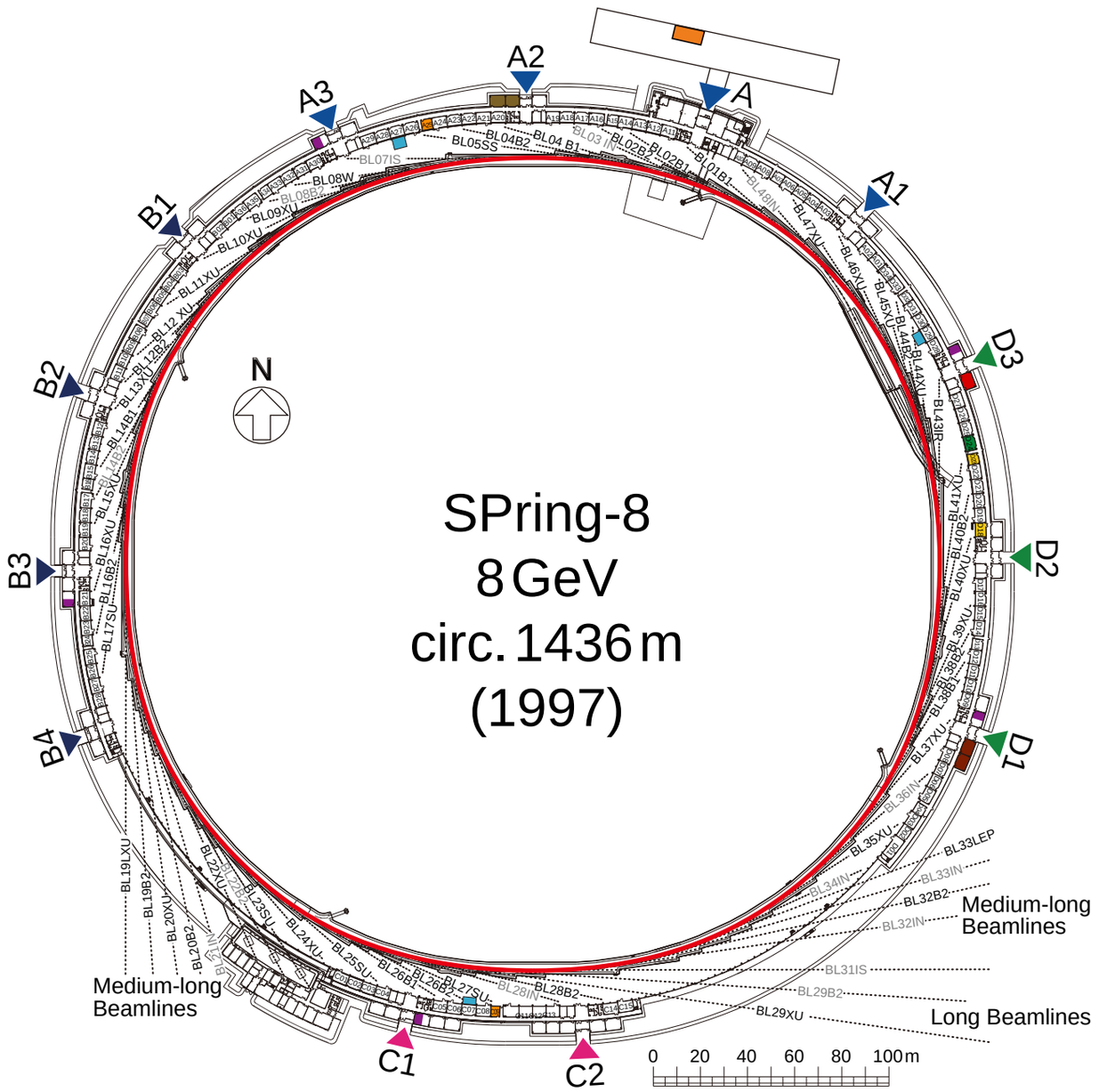
A compact synchrotron facility, AichiSR



AichiSR & SPring-8



AichiSR
1.2 GeV
circ. 72 m
(2012)

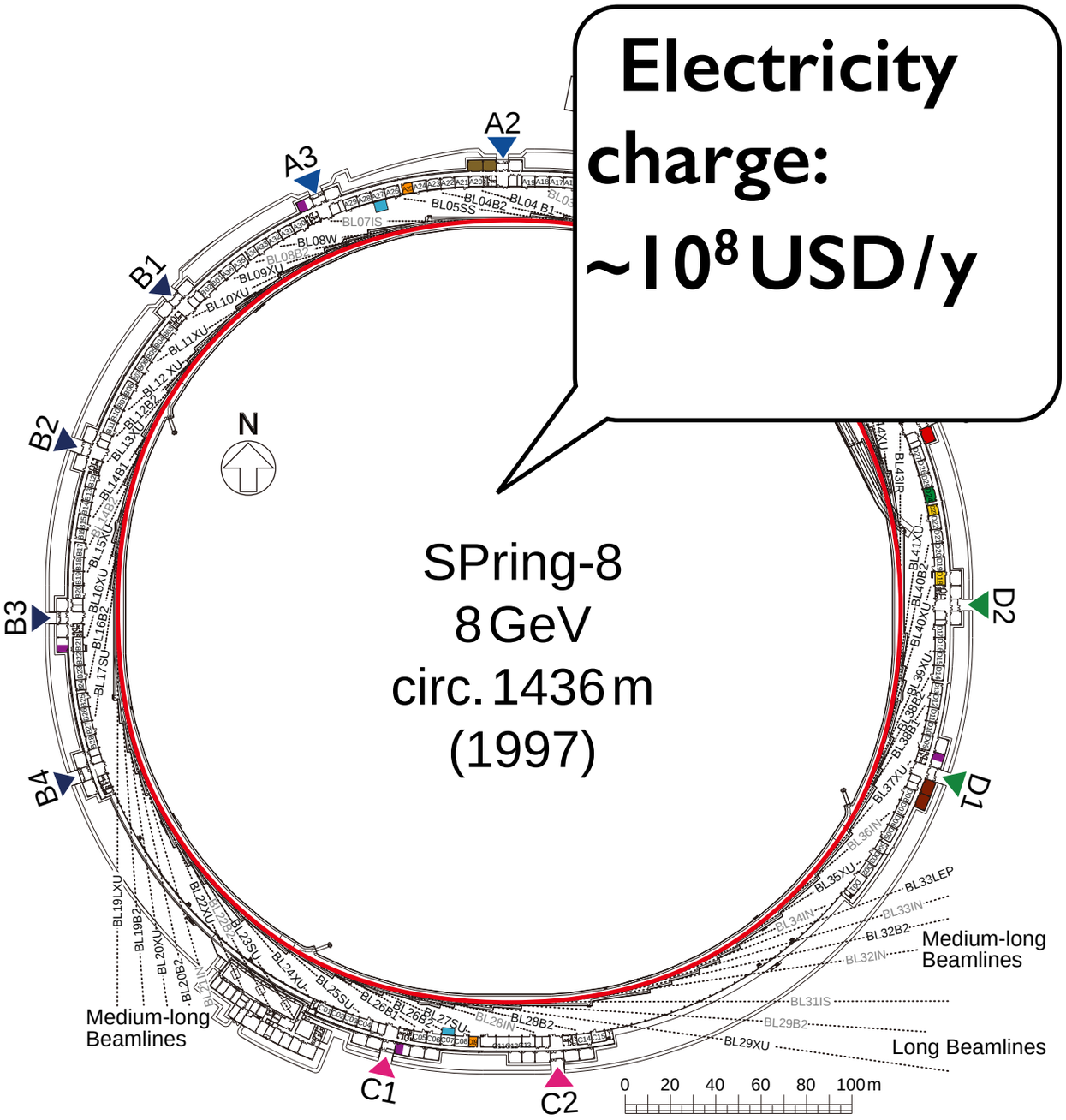


AichiSR & SPring-8

Electricity charge: $< 10^6$ USD/y

AichiSR
1.2 GeV
circ. 72 m
(2012)

Electricity charge: $\sim 10^8$ USD/y

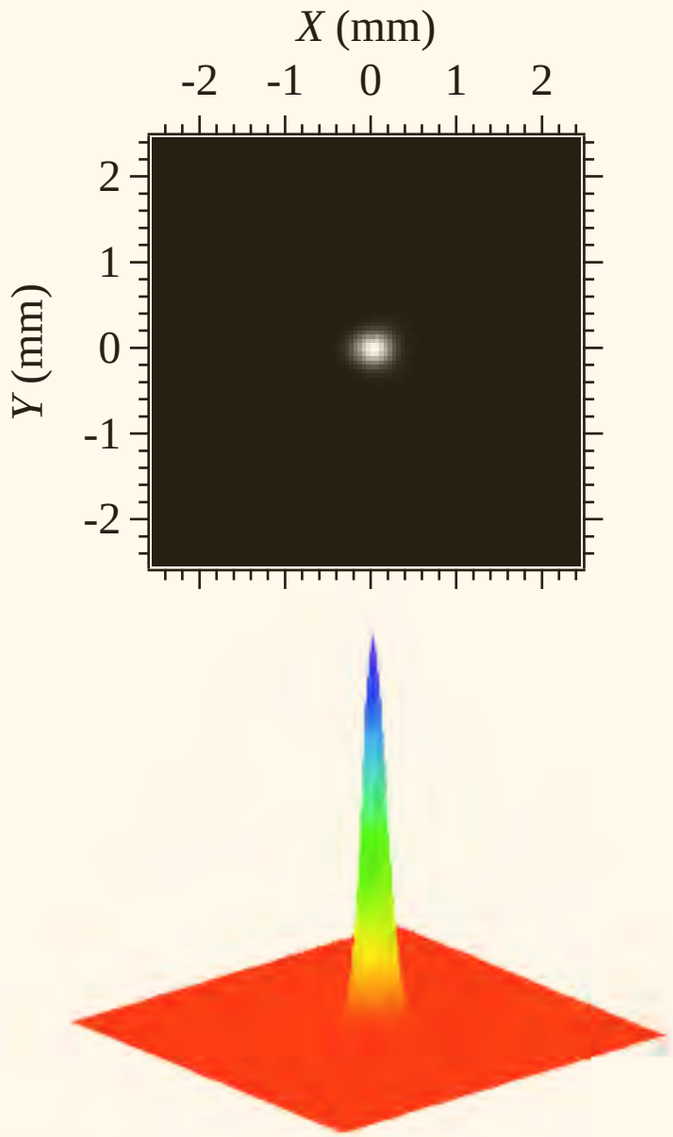


AichiSR & SPring-8 PXRD BLs for industrial use

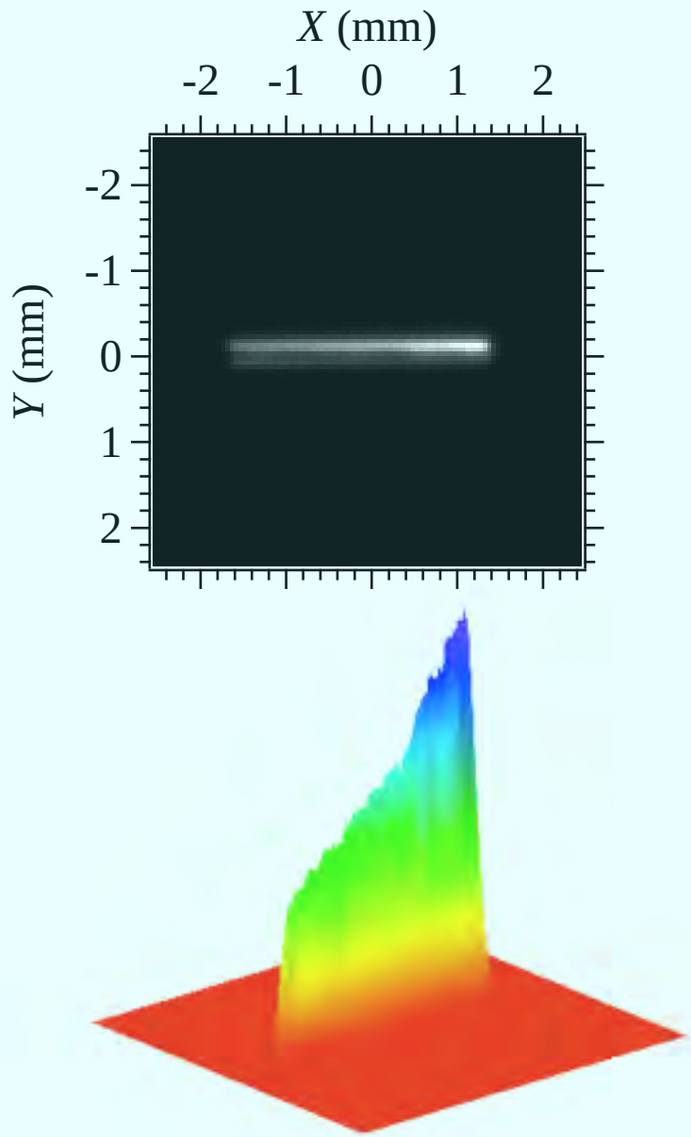
	AichiSR BL5S2	SPring-8 BL19B2
Light source	superconducting bending magnet ~ 5T	normal bending magnet ~ 0.679T
Photon energy	5 ～ 23 keV	5 ～ 72 keV
Photon flux	1.4×10^{11} photons / s @ 12 keV (1 Å)	～10^{9} photons / s
Resolution (E / ΔE)	7,000 @ 12 keV	～10,000
Beam size	Width 0.35 mm Height 0.21 mm	Width 2.5 mm Height 0.14 mm

AichiSR & SPring-8 PXRD BLs for industrial use

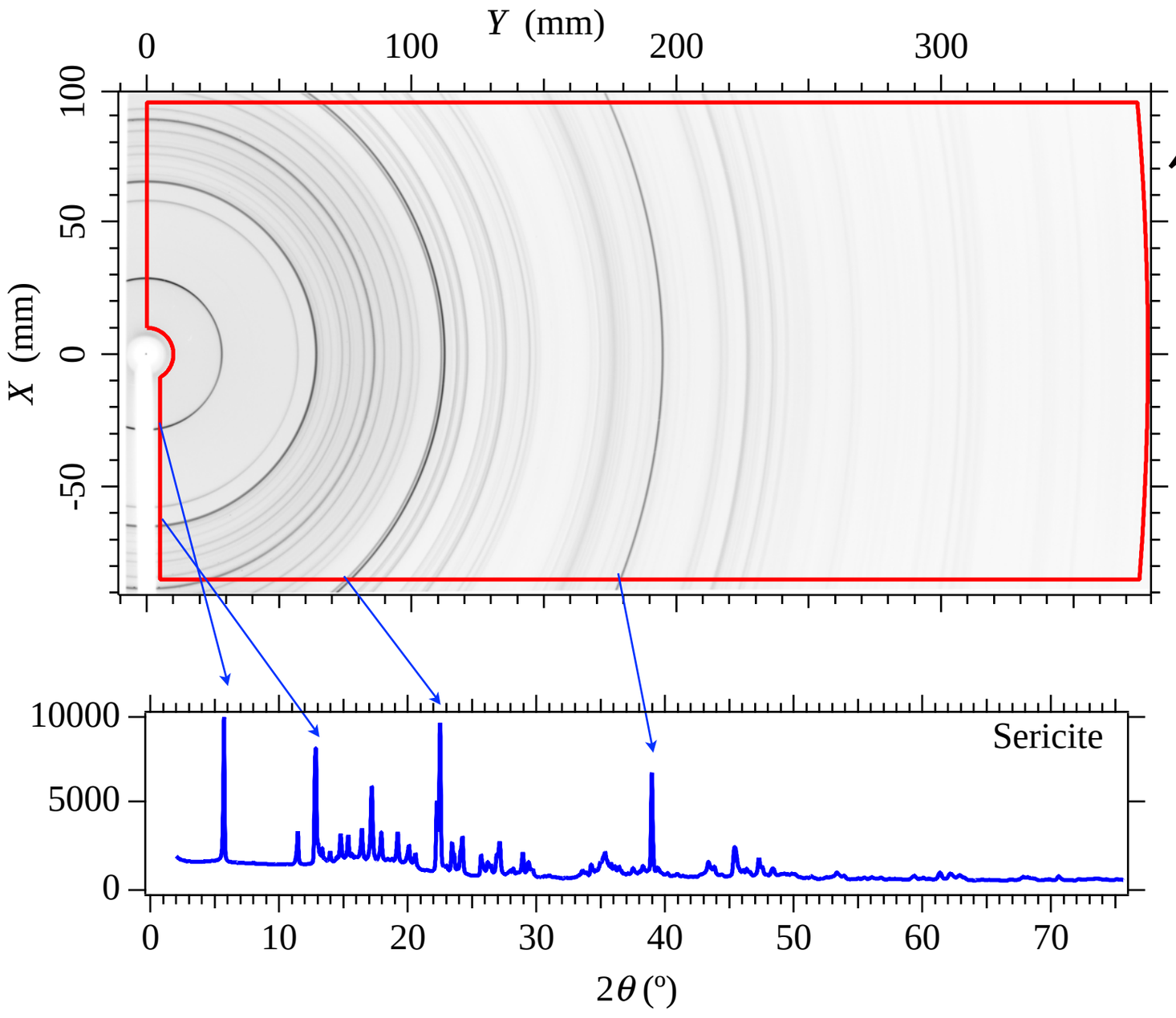
AichiSR BL5S2



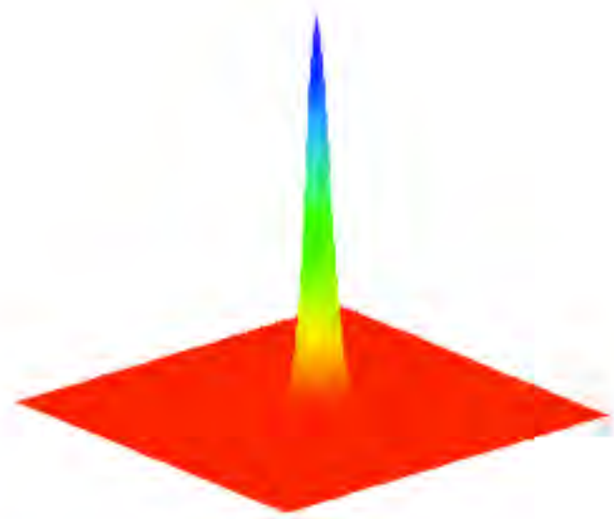
SPring-8 BL19B2



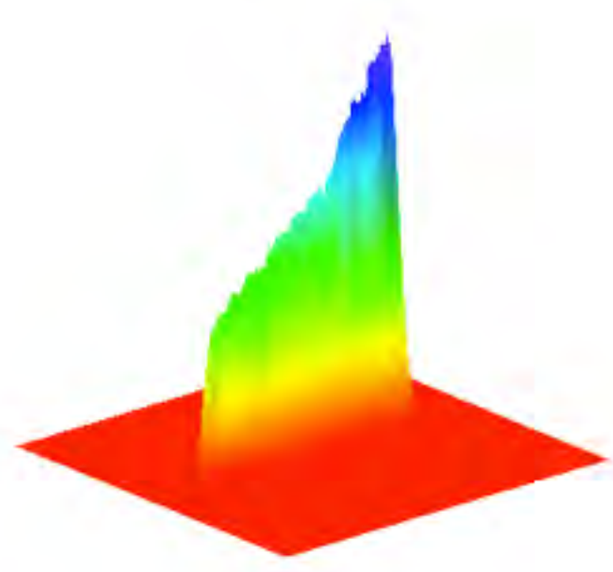
Debye-Scherrer image



Sensitivity x 80

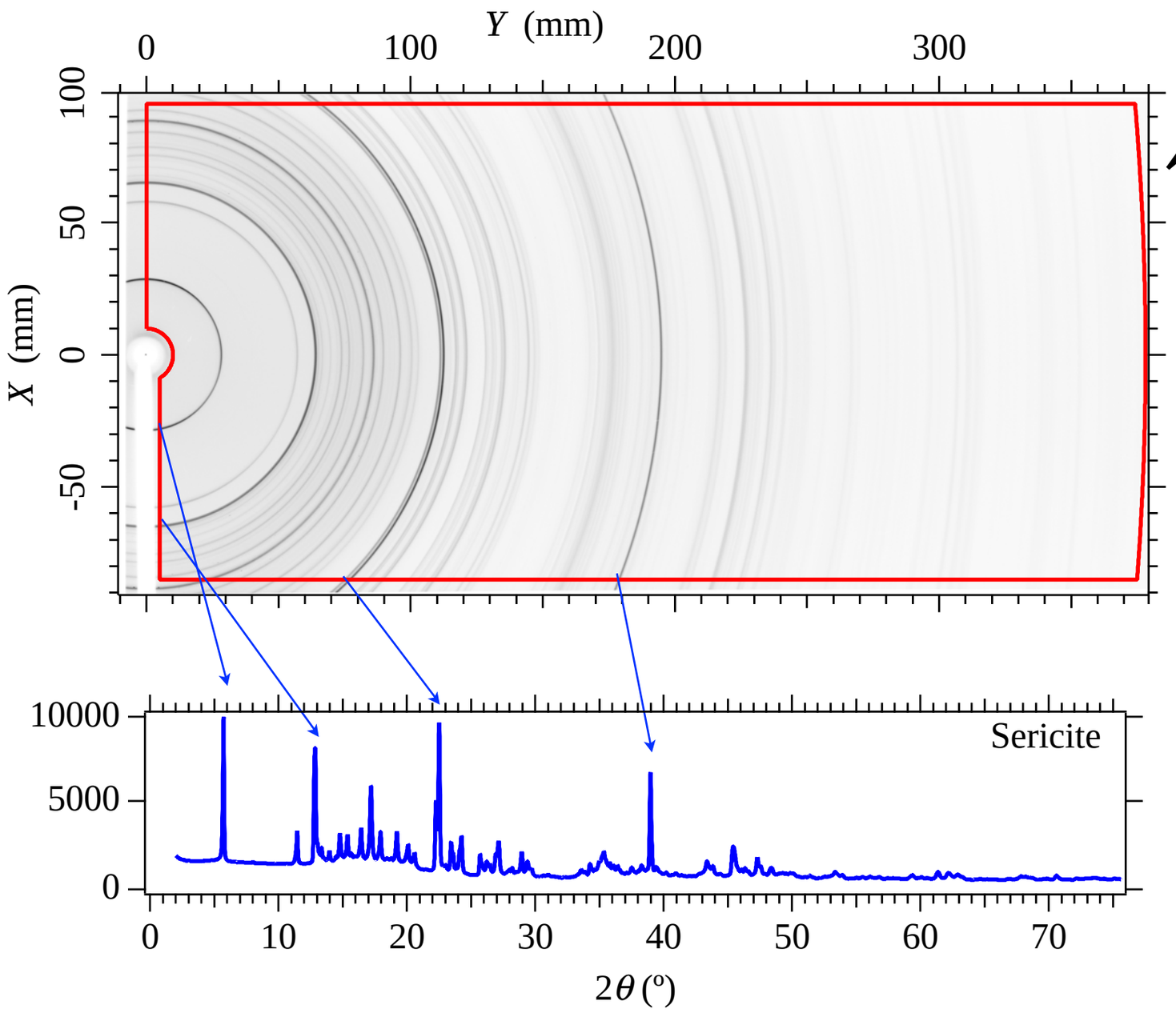


AichiSR BL5S2

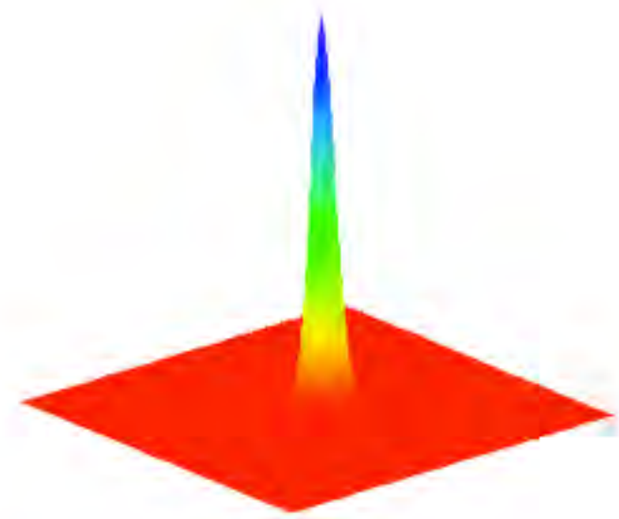


SPring-8 BL19B2

Debye-Scherrer image



Sensitivity x 80



AichiSR BL5S2

No axial-divergence aberration
Increased number of diffracting crystallites

Fees

Beam-time fee of AichiSR:
40,000 JPY (400 USD) / h for industrial use
20,000 JPY (200 USD) / h for academic use

NIS Co-Chair report (2014 – 2015)

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18th Reactivity of Solids

9-13 June 2014, St. Petersburg

Sponsored by the ICDD

137 participants from 18 countries: 6 plenary lectures, 18 invited talks, 37 oral and 93 poster presentations

The ICCD booth was exhibited

18th Reactivity of Solids

9-13 June 2014, St. Petersburg

At the ICDD booth

Scott Misture lecture

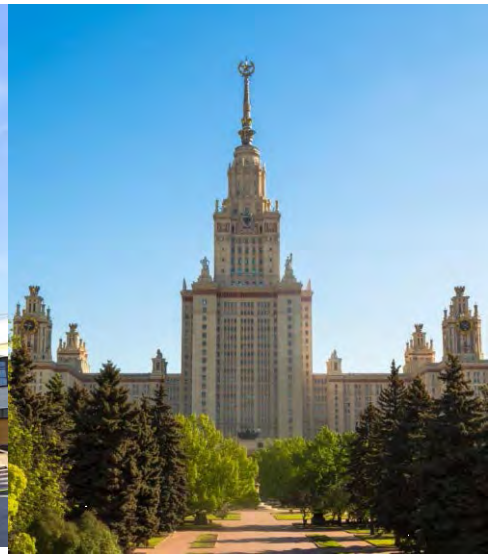
INTERNATIONAL REPORT

Solid Energy: a Report on the 18th International Symposium on the Reactivity of Solids

O. Levin,[1] S. Kazakov,[2] and E. Antipov[2]

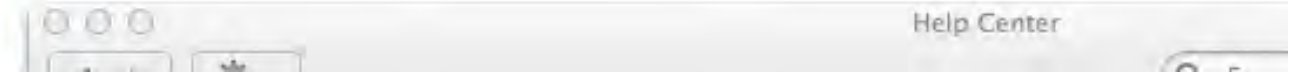
Powder Diffraction 29 (4), December 2014

July ~~13-18 2014~~, Moscow
XII International Conference on Nanostructured Materials (NANO-2014)



Professor **Tim G. Fawcett**, International Centre for Diffraction Data (USA)

Title of lecture: "The Analysis of Nanomaterials by Powder Diffraction"



Sponsored by the ICDD/ ICDD booth

About 1000 participants from 57 countries/ 268 students.

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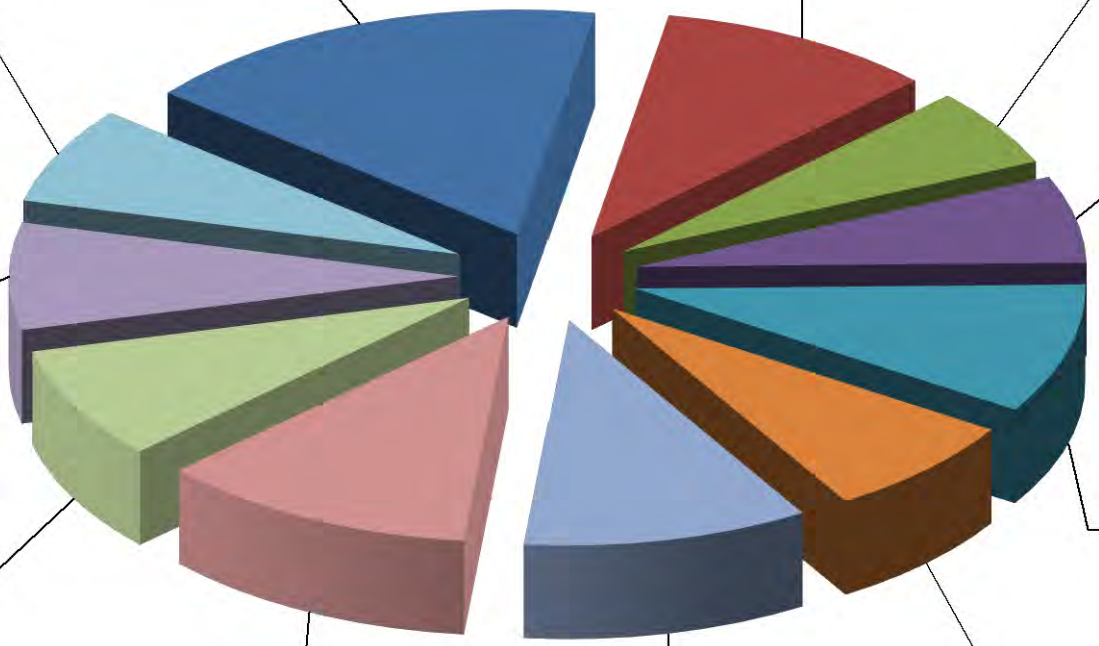
NANO 2014 Sessions



Session 01: Formation, Shaping and Self-assembly of Inorganic Nanoparticles; Carbon Nanomaterials

Session 02: Thin Films and Heterostructures, 2D and 3D Nanofabrication

Session 03: Nanoceramics

Session 04: Bulk Metallic Nanomaterials

Session 05: Nanocomposites and Hybrid Nanomaterials

Session 06: Polymer, Organic and Other Soft Matter Materials

Session 07: Nanomaterials for Energy

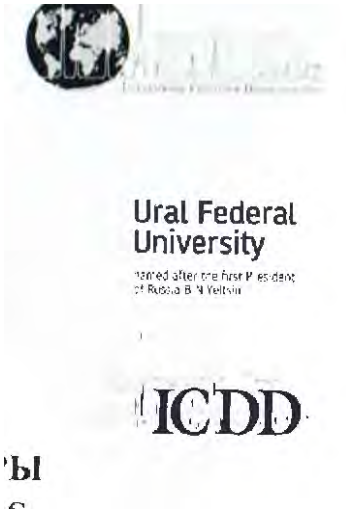
Session 08: Biological and Biomedical Nanomaterials

Session 09: Nanomaterials: Mechanics and Applications in Mechanical Engineering

Session 10: Nanomaterials for Information Technologies, Ianoelectronics and Nanophotonics

Session 11: Nanomaterials and Catalysis

XVIII International Conference on Crystal Chemistry, XRD & Spectroscopy of Minerals (Ekaterinburg, Russia), 13-15.10.2014



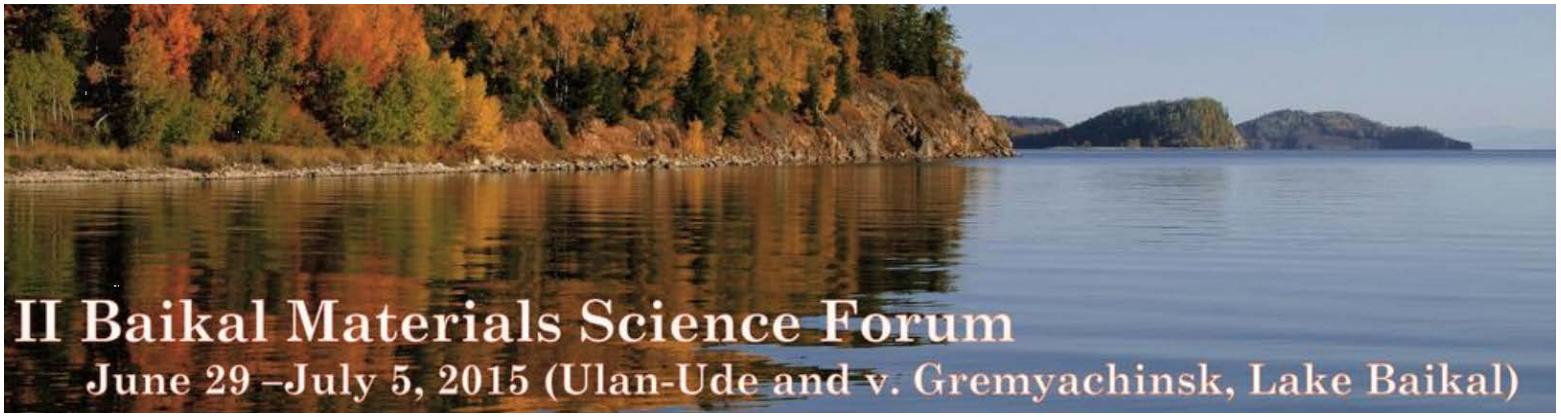
Sponsored by ICDD

ICDD booth

The total amount of the participants was 113:
Russia (106), Ausria (4), Ukraine (2), Azerbajan (1)
20 young scientists have been supported

Activities for 2015/16

1) 2nd Baikal Materials Science Forum

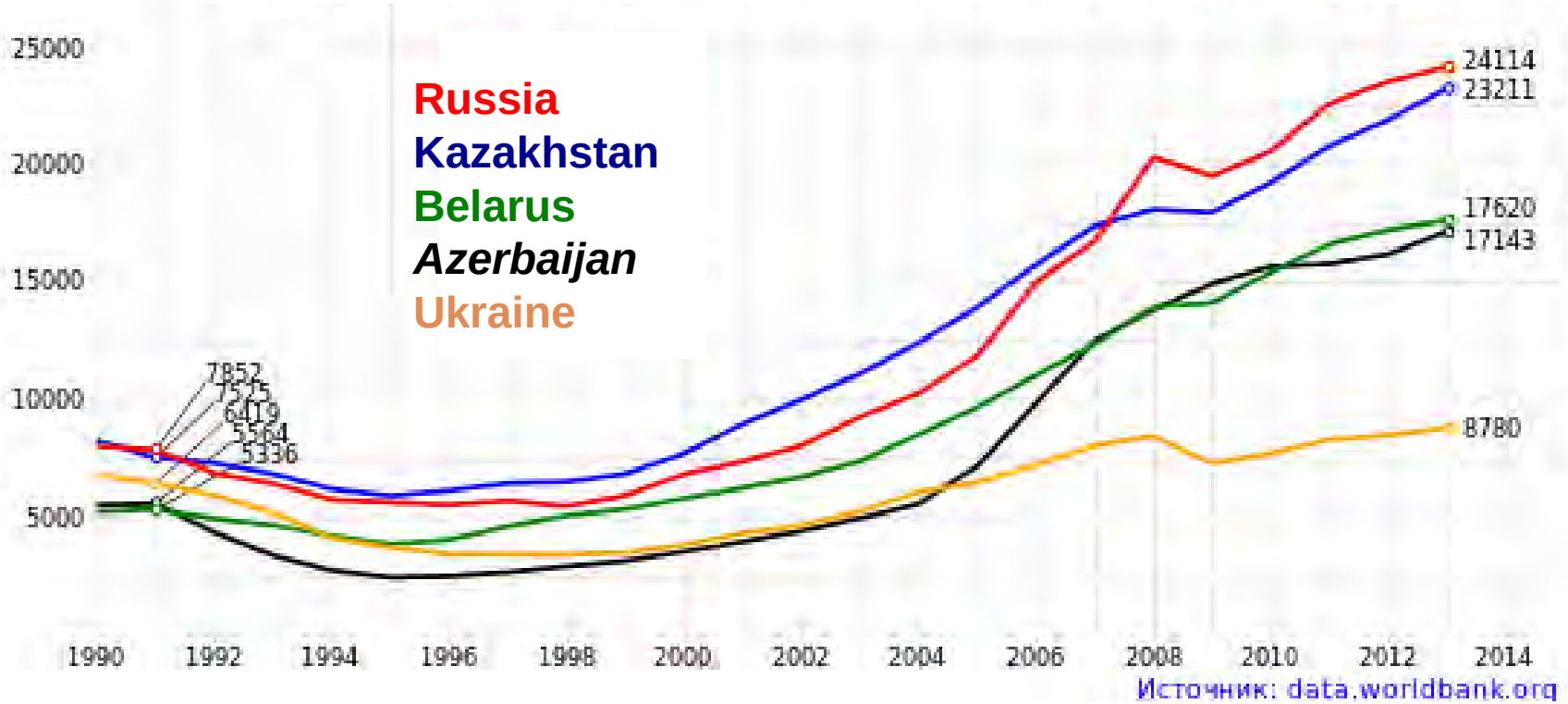


2) ICDD workshop in Baku (Azerbaijan) – ?
Local organizer – Bogdan Lazoryak

3) Activity in Kazakhstan?

4) ICDD membership

GDP per capita in some former SU countries



Ruble/ US $ ratio variation

Report of the Technical Regional Co-Chair – North America –

March 2015

John Anzelmo

North American Meetings

Key Exhibits & Educational Events • FY 2014-15

Materials Research Society (MRS Spring 2014)
San Francisco, CA • 21 - 25 April 2014

Denver X-ray Conference (DXC)
Big Sky, MT • July 28 – 1 August 2014

Microscopy & Microanalysis (M&M)
Hartford, CT • 3-7 August 2014

23rd IUCr Congress and General Assembly (IUCr 2014)
Montreal, Canada • 5 - 12 August 2014

XXI International Materials Research Congress (IMRC 2014)
Cancun, Mexico • 17 - 21 August 2014

Materials Science & Technology (MS&T 2014)
Pittsburgh, PA • 12 - 16 October 2014

Geological Society of America (GSA)
British Columbia, Canada • 19 - 22 October 2014

American Association of Pharmaceutical Scientists (AAPS)
San Diego, CA • 2 - 6 November 2014

Materials Research Society (MRS)
Boston, MA • 30 November - 5 December 2014

ICDD Clinics and Workshops North America

ICDD Clinics - North America

- **Practical X-Ray Fluorescence Clinic**
  28 April – 2 May 2014
  Newtown Square, PA
  Eileen Jennings, Steph Jennings, Terry Maguire, Denise Zulli

- **Fundamentals of X-Ray Powder Diffraction Clinic-XRD I**
  2-6 June 2014
  Newtown Square, PA
  Eileen Jennings, Steph Jennings, Terry Maguire, Denise Zulli

- **Advanced Methods in X-Ray Powder Diffraction Clinic-XRD II**
  9-13 June 2014
  Newtown Square, PA
  Eileen Jennings, Steph Jennings, Terry Maguire, Denise Zulli

ICDD Workshops – North America

- **Rietveld Refinement & Indexing Workshop-Basic Workshop**
  29 September - 1 October 2014
  Newtown Square, PA
  Eileen Jennings, Steph Jennings, Terry Maguire, Denise Zulli

- **Rietveld Refinement & Indexing Workshop-Advanced Workshop**
  2-3 October 2014
  Newtown Square, PA
  Eileen Jennings, Steph Jennings, Terry Maguire, Denise Zulli

- **PDF Users' Meeting at DXC**
  27 July 2014
  Big Sky, Montana

REGIONAL CO-CHAIR: South America
2014 - 2015

Miguel Delgado

International Union of Crystallography
Commission on Mathematical and Theoretical Crystallography

International School on Fundamental Crystallography

Fourth MaThCryst School in Latin America
27 April - 10 May, La Plata, ARGENTINA

Prof. Gustavo Echeverría
Universidad Nacional de La Plata
http://www.crystallography.fr/mathcryst/laplata2014.php

Invited Instructors:

Mois I. Aroyo (Spain), Ernesto Estévez Rams (Cuba), Massimo Nespolo (France), Leopoldo Suescun (Uruguay), Lee Daniels (Agilent-USA)

Local Instructors:

Ana Bianchi, Susana Conconi, Gustavo Echeverría, Raimundo Lora Serrano, Gustavo Pozzi.

Sociedad Mexicana de Cristalografía A.C. SMCr

Séptimo Congreso Nacional de la SMCr
(VII National Crystallography Congress)
4 – 9 May 2014, Villahermosa, Tabasco, MEXICO

Centro Internacional de Vinculación y Enseñanza (CIVE),
Universidad Juárez Autónoma de Tabasco

Crystallite Size Characterization in Nanomaterials

Invited Lecture: Miguel Delgado
(*Demo of PDF-4+*)

XXIII INTERNATIONAL MATERIALS RESEARCH CONGRESS 2014

17 – 21 August, Cancun, Mexico

Sociedad Mexicana de Materiales

The Materials Research Society (MRS)

WORKSHOP

- Tom Blanton (ICDD)
- Lauro Bucio (UNAM)
- Miguel Delgado (ICDD/ULA)

Tom Blanton -Invited Speaker-
Symposium 5B. Structural and Chemical Characterization of Metal Alloys and Compounds

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Rigaku OpenLab Colombia

27 – 31 October 2014

Universidad Industrial de Santander (UIS)

Bucaramanga – COLOMBIA

Prof. José Antonio Henao

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XIV Latin American Seminar of Analysis by X-Ray Techniques 2014 - Carlos Paz (Argentina)

SARX-2014

XIV Seminario Latinoamericano de Análisis por Técnicas de Rayos-X

November 3 – 7, 2014

Carlos Paz, Córdoba, ARGENTINA

PLENARY LECTURE

"Tools and References for the Analysis of Nanomaterials"

Tim Fawcett

INVITED LECTURES

"The Analysis of Pharmaceutical Materials using the Powder Diffraction File"

Graciela Delgado

"The Analysis of Modulated Strructures using the Powder Diffraction File"

Miguel Delgado

WORKSHOP

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International Workshop

Characterization of Materials using X-ray Powder Diffraction

23 – 27 June 2014
Mérida-VENEZUELA

Invited Instructors:

- Bob Von Dreele
- Jim Kaduk
- Matteo Leoni

In a joint effort of the Colombian and Venezuelan Societies of Crystallography, two courses on X Ray Diffraction Techniques are being organized: a course on X ray Powder Diffraction which will take place in Mérida, Venezuela, from June 23 to 27 of 2014, and a course on Single Crystal X-Ray Diffraction which will take place in Bucaramanga, Colombia, in September.

Universidad de Los Andes
Facultad de Ciencias
Departamento de Química
Mérida - Venezuela

Curso

Caracterización de Materiales Policristalinos mediante Técnicas de Difracción de Rayos X

23 al 27 de Junio de 2014

Evento Colombo-Venezolano organizado en ocasión del Año Internacional de la Cristalografía (IYCr 2014)

Laboratorio de Cristalografía-*LNDRX*
(Universidad de Los Andes)

Laboratorio de Difracción de Rayos X
(Universidad Industrial de Santander)

Contacto: Prof. Miguel Delgado
Telf.: 58-274-2401372
correo-e: migueld@ula.ve

NEXT EVENTS:

XXIII International Materials Research Congress (IMRC)

August 16-20, 2015

Cancun, Mexico

ICDD WORKSHOP in

Symposium 6G

Materials Science of Pharmaceutical Solids

Dr. Tom Blanton, ICDD, USA
Prof. Lauro Bucio, UNAM, Mexico
Prof. Miguel Delgado, ULA/ICDD, Venezuela

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XXII Reunião da ABCr
I Reunião da LACA

9 a 11 de setembro de 2015

Convidamos a todos os cristalógrafos dos países latinoamericanos a participar desta importante Reunião com a qual a LACA inicia sua atuação como membro Regional da União Internacional de Cristalografia.

Local da Reunião

Instituto de Física,
USP, São Paulo, Brasil

Comissão Organizadora Internacional

Marcia C. A. Fantini (Brasil)
Diego G. Lamas (Argentina)
Mauricio Fuentealtaba (Chile)
José Roberto Vega-Baudrit (Costa Rica)
José Antonio Henao (Colombia)
Graciela D. Delgado (Venezuela)
Lauro Bucio Galindo (México)
Alejandro Buschiazzo (Uruguay)
Iris C.L. Torriani (Brasil) – Chair

"Workshop" satélite: "High Pressure Crystallography" 12-14 de set. 2015, Laboratório Nacional de Luz de Síncrotron – LNLS - Campinas, SP, Brasil

O programa científico completo *(em elaboração)* será divulgado no segundo anuncio do encontro.

Contactos:
laca.cristalografia@gmail.com - mfantini@if.usp.br - torriani@ifi.unicamp.br

Possible GiA Workshop
8 September 2015
USP – Sao Paulo, BRAZIL

UNIVERSIDADE FEDERAL
DE SANTA CATARINA

III School of Advanced Studies in Crystallization and Crystallography for Latin America
(ECRISLA 2015)

December 7 – 18, 2015
Florianópolis Brazil

- Module 1: Crystallization (December 7 - 11)
- Module 2: Crystallography (December 14 – 18)

Prof. Carlos E.M. Campos – Prof. Silvia Cuffini

Regional Co-Chair's Report for the United Kingdom & Ireland

David Rendle

Activities since March 2014

- BCA Spring Meeting April 7th – 10th, 2014 held at Loughborough University
- XRF Meeting (Joint BCA/RSC Atomic Spectroscopy Meeting), June 18th 2014 Leicester University
- BCA Industrial Group Autumn Meeting November 12th, 2014 held at the Royal Institution of Great Britain, London

BCA Spring Meeting 2014

"Crystallography @ 100: Looking to the future, learning from the past"

- Lonsdale Lecture: Henry Chapman (DESY)
  "Macromolecular Crystallography with X-ray laser pulses"

- Bragg Lecture: Judith Howard FRS (Durham University)
  "Exploring a century of reciprocal space: same old theory – endless new results"

BCA Meeting (contd): Plenary lectures

- Paul Raithby (University of Bath)

"Understanding the solid state into the next 100 years"

- Joel Bernstein (NYU, Abu Dhabi)

"Crystallography @100: Learning from the past and trying to look into the future"

XRF Meeting June 18th, 2014
(Joint BCA/RSC Atomic Spectroscopy Meeting)

- Workshop on handheld XRF instruments

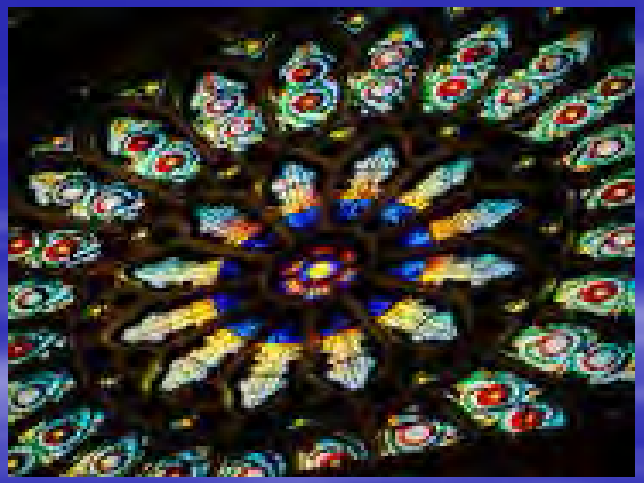
- User presentations (handheld and conventional instruments)

Dave Taylor (Chair)
Kevin Solman (Plymouth Univ.)
David Beveridge
Ros Schwarz

Prize for the most unusual XRF sample

- Dave Taylor's 1g sample of medieval glass from the Rose Window of York Minster – contains more K & Ca than modern soda glass

York Minster



Rose Window

Afternoon Session

- Workshop on benchtop/portable XRF instruments

- Mathieu Bouchard – calibration strategies in Cement Industry
- Andy Scothern – Micro XRF – EDX/SEM combination
- Garry Smith – Internal standards for Quantitative XRF

Mathieu Bouchard
Andy Scothern
David Beveridge (Chair)
Garry Smith

BCA IG Autumn Meeting November 12th, 2014

"2014 International Year of Crystallography Celebration Meeting"

The Royal Institution of Great Britain, London

- Andy Doré (Heptares Therapeutics) "ABC of G-protein coupled receptor structural biology (3D talk)"

- Michael Probert (Newcastle University) "High pressure – the polymorph playground"

- Chris Frampton (Brunel University) "Structural studies at the salt-cocrystal interface"

Forthcoming activities

- BCA Spring Meeting March 30th – April 2nd, 2015 to be held at York University
- BCA XRF Group Meeting June 17th, 2015 to be held at Leicester University
- 12th International Conference on Materials Chemistry (MC12) July 20th – 23rd 2015 to be held at York University

Still a United Kingdom? Just!

- Outcome of the Scottish Independence vote:

- Yes – 45% (1,617,989)
- No – 55% (2,001,926)

- Turnout: 84.6%

UK General Election
May 7th, 2015

House of Commons: 650 Members of Parliament (MPs)

2010 result: Conservative 307, Labour 258, Lib Dem 57, Other 28

Coalition between Conservatives & Liberal Democrats

59 Scottish MPs are in Parliament at present

Labour 41
Conservative 1
Liberal Democrats 11
SNP 6

Possible outcomes of May 7th

David Cameron
Conservative

+

Nicola Sturgeon
Scottish National Party

Possible coalition or "informal arrangement"?

+

Ed Miliband
Labour

As the ancient saying (or curse) goes – "May you live in interesting times!"

When Boris met Hillary

Boris Johnson (Mayor of London) visits Boston, New York & Washington in February 2015

Back to the future? A vision of the year 2020?